# Optimal configuration of a class of irreversible heat engines. II

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In a previous paper we analyzed a class of irreversible cyclic heat engines to find their optimal operating configuration for specific performance goals. In that paper the thermodynamic variables of the working fluid were not treated as dynamical variables, instead the dynamics was replaced by an integral constraint. In this paper we reanalyze the same class of heat engines treating the thermodynamic variables of the working fluid as dynamical variables, and we obtain the optimal configuration of the engine when the performance goal is to maximize the average power output per cycle or, alternatively, to maximize the efficiency of the engine. To carry through this program it is necessary to use mathematical techniques from optimal-control theory. Since this subject is unfamiliar to most physicists and chemists, we briefly introduce some of the central ideas of the theory.

# I. INTRODUCTION

In the preceding paper,<sup>1</sup> we analyzed a subclass of cyclic endoreversible engines. Endoreversible engines were defined as heat engines with working fluids that undergo reversible transformations and irreversible processes, if they occur, occur only due to the interaction between the engine and its environment. The objective of the analysis was to obtain the best operating configuration for the engines consistent with a given set of constraints and a specific operating goal.

The subclass of engines studied in Ref. 1 was characterized by the requirement that the irreversible interaction between the engines and the environment was (linear) heat conduction. For these engines two operating goals were considered, each goal was formulated in terms of a maximum principle and the calculus of variations was used to obtain the best operating configuration.

In this paper we will not be able to use the calculus of variations in its standard form but must instead use optimal-control theory. The reason for this is that in this paper we wish to treat the thermodynamic variables describing the working fluid as dynamical variables. In Ref. 1, the working fluid was characterized explicitly by its temperature and implicitly by a second independent variable, for example, its volume. Since the volume did not appear explicitly in the equations, it was possible to solve the maximization problem without using dynamical equations for the thermodynamic variables of the working fluid. It was . simply assumed that the volume could be adjusted appropriately to give the desired solution. In this paper we reanalyze the heat engines studied in Ref. 1 including the dynamical equations for the thermodynamic variables of the working fluid. These equations complicate the analysis and lead us to the use of optimal-control theory.

Optimal-control theory<sup>2-6</sup> has been developed and used widely by engineers and mathematicians in the last 25 years, however, the subject does not appear to have been used in the analysis of fundamental physics problems.<sup>9</sup>

The plan of this paper is as follows. In Sec. II we define our model heat engine and formulate the problem we wish to solve. In Sec. III we solve the problem formulated in Sec. II and in doing this introduce some techniques from optimal-control theory. In Sec. IV, we discuss the solution obtained in Sec. III and make contact with the results of Ref. 1. Finally in Sec. V, we summarize our results and draw some conclusions from this work.

#### II. MODEL HEAT ENGINE

We briefly define the model heat engine, referring the reader to Ref. 1 for more details. The engine is a standard engine with a cylinder and piston which is used to do work on the outside world. The engine operates cyclically subject to the following restrictions:

(i) The engine is endoreversible.

(ii) The walls have a constant thermal conductivity  $\rho$ , however, walls are available such that  $\rho$ may take on any value such that  $0 \le \rho \le \rho_0$ .

(iii) When the engine is in thermal contact with a heat reservoir of absolute temperature  $T_R$ , the heat flux into the working fluid is given by a linear law

$$\dot{q} = \rho(T_R - T), \tag{2.1}$$

where T is the absolute temperature of the work-

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ing fluid.

(iv) Each thermal reservoir has a constant temperature  $T_R$  where

 $T_L \leq T_R \leq T_H.$ 

(v) The work done by the engine in one cycle is given by

$$W = \int_0^\tau P \dot{V} dt, \qquad (2.2)$$

where P and V are the pressure and volume of the working fluid, the time derivative of V is denoted by  $\dot{V}$ , and  $\tau$  is the cycling period of the engine.

(vi) The working fluid is a perfect gas, i.e., an ideal gas, with constant heat capacities.

Assumptions (i)-(v) are the same, with one exception, as those of Ref. 1. The exception is in (ii) where we allow  $\rho$  to be a variable whose value is determined by the performance goal. Assumption (vi) was unnecessary in Ref. 1, but it is necessary to know the equation of state of the fluid to treat the dynamics of the working fluid. We have selected the simplest equation of state so that our calculations can be done analytically. A seventh assumption will be added below.

In order to put Eqs. (2.1) and (2.2) into the form that will be useful for our calculation we use the first law of thermodynamics for a perfect gas:

$$C_V \dot{T} + C_V (\gamma - 1) T \dot{V} / V = \dot{q},$$
 (2.3)

where  $C_V$  is the constant-volume heat capacity of the gas in the cylinder,  $\gamma$  is the ratio of the heat capacity at constant pressure and  $C_V$ , and a dot over a variable always means the time derivative. Substituting Eq. (2.1) into (2.3) and defining some new variables we have

$$\dot{T} = -cT + \hat{\rho}(T_R - T), \qquad (2.4)$$

$$\beta \equiv (\gamma - 1) \ln(V/V_0), \qquad (2.5)$$

$$\dot{\beta} = c, \qquad (2.6)$$

where  $\hat{\rho} = \rho/C_V$  and  $V_0$  is a constant reference volume. In terms of these variables Eq. (2.2) becomes

$$W = C_V \int_0^\tau cT \, dt. \tag{2.7}$$

The reason for introducing the variables  $\beta$  and c will become clear in Sec. III when we outline the method for solving our problem. Finally we note that the input energy is given by

$$Q_1 = C_V \int_0^{\tau} \hat{\rho} (T_R - T) \theta (T_R - T) dt, \qquad (2.8)$$

where  $\theta(x)$  is the Heaviside step function,  $\theta(x) = 1$  if x > 0 and  $\theta(x) = 0$  if x < 0.

Our problem is to determine  $\hat{\rho}(t)$ ,  $T_R(t)$ , and

c(t) so that either case (A) the average power output is a maximum or case (B) the efficiency is a maximum for a given value of  $Q_1$ . These are the same problems we solved in Ref. 1, however, in this paper we must ensure that the dynamical equations (2.4) and (2.6) are satisfied. In order to obtain physically sensible results we must restrict the variable c which is a constant times the fractional rate of change of the volume of the cylinder. Thus we add a seventh assumption:

(vii) Let  $c_m$  and  $c_M$  be arbitrary constant positive numbers. Then we require that c(t) be restricted such that

$$-c_m \leq c \leq c_M. \tag{2.9}$$

This completes the specification of the model heat engine. We now present the mathematical techniques that will be used to solve problems (A) and (B).

## III. OPTIMAL CONTROL THEORY (REFS. 2-6)

In the 25 years since its founding, mathematicians and engineers have steadily increased the range of systems that can be studied using optimal-control theory. We are interested in a particularly simple type of system and will limit our discussion accordingly.

## A. Some definitions of terminology

A system is an object whose state at any time is characterized by a set of n real numbers  $x_1, \ldots, x_n$ which may be visualized as a vector  $\vec{x}$  in an n-dimensional Euclidean vector space. The system is assumed to have *controls* described by m real numbers  $u_1, \ldots, u_m$  whose values influence the evolution of the state of the system in a way to be specified below. The controls may be visualized as vectors  $\vec{u}$  in a m-dimensional Euclidean vector space. We are particularly interested in the case in which the *admissible controls* are limited to a closed, bounded region of this space.

The systems that we are interested in are (differential) dynamical systems<sup>6</sup> by which we mean that the state of the system  $\vec{\mathbf{x}}(t)$  at time  $t > t_0$  is uniquely determined by a set of differential equations

$$\vec{\mathbf{x}}(t) = \vec{\mathbf{F}}[\vec{\mathbf{x}}(t), \vec{\mathbf{u}}(t)]$$
(3.1)

and initial conditions  $\vec{\mathbf{x}}(t_0)$ , where  $\vec{\mathbf{F}}[\vec{\mathbf{x}},\vec{\mathbf{u}}]$  and  $\partial \vec{\mathbf{F}}[\vec{\mathbf{x}},\vec{\mathbf{u}}]/\partial x_j$  are continuous vector functions of  $\vec{\mathbf{x}}$  and  $\vec{\mathbf{u}}$ , and  $\vec{\mathbf{u}}(t)$  is a piecewise continuous vector function whose values are admissible controls.

In the problem formulated in Sec. II, T and  $\beta$  are the state variables and  $T_R$ ,  $\hat{\rho}$ , and c are the control variables. The equations of motion (2.4) and

(2.6) with

$$F_1 \equiv -cT + \hat{\rho}(T_R - T) \tag{3.2}$$

and

 $F_2 \equiv c \tag{3.3}$ 

generate a vector function  $\vec{F}$  which satisfies the requirements of a dynamical system.

Our system is special in several ways. For example,  $\overline{F}$  does not depend on time explicitly: such systems are called *autonomous*. Our system has no memory, that is, the evolution of the system for  $t > t_1$  (>  $t_0$ ) depends only on  $\mathbf{x}(t_1)$  and  $\mathbf{u}(t)$  for  $t > t_1$ . There are no constraints on our state variables, in general state constraints, which may take the form of equality constraints  $\vec{S}[\vec{x}] = \vec{0}$  or inequality constraints  $\vec{S}[\vec{x}] \ge \vec{0}$ , greatly complicate the problem of finding an optimal solution. Of course, the state variable T is constrained to be positive (note  $\beta$  is not, although  $V \ge 0$ ) but this presents no real difficulty since the optimal solution will require  $T > T_L$ . Another important special feature of our problem is that the controls are noninertial, that is, they may change discontinuously. For example, c which controls the rate of expansion of the volume of the cylinder may change instantaneously from its maximum to its minimum value at the whim of the controller. In a real system there is always a lag due to the inertia of any movable part, this may be taken into account by making c continuous but we will no do so.

Next we define a *performance index* or *cost functional* which specifies the operating goal of the system,

$$I = G(\mathbf{\bar{x}}_{1}, t_{1}) + \int_{t_{0}}^{t_{1}} L[\mathbf{\bar{x}}(t), \mathbf{\bar{u}}(t)]dt$$
(3.4)

where  $\vec{\mathbf{x}}_1 = \vec{\mathbf{x}}(t_1)$  is the final state of the system. In our case we have  $G \equiv 0$  and either I = W or I = W $- \mu Q_1$  depending on whether we are maximizing the average power output or efficiency. In the latter case the constancy of  $Q_1$  is a constraint.

## B. Statement of the optimal control problem

The optimal control problem requires us to find an admissible control  $\vec{u}^*(t)$  such that the system is driven from its initial state to its final state in the manner that maximizes the performance index. Such a control is called an *optimal control* and the phase space trajectory  $\vec{x}^*(t)$  is called an *optimal trajectory*.

There are obviously a wealth of problems that fit this definition. In the cases discussed in this paper the initial and final state are the same and the time for one cycle is fixed. Problems in which the system is periodic do not seem to have been much discussed in the mathematical literature.

#### C. Pontryagin maximum principle

We will now state the Pontryagin maximum principle which provides a set of necessary conditions for solving the optimal-control problem (this is often stated in the literature as a minimum principle). First we define the Hamiltonian  $H(\vec{\mathbf{x}}, \vec{\mathbf{u}}, \vec{\psi})$  by

$$H(\vec{\mathbf{x}},\vec{\mathbf{u}},\vec{\psi}) \equiv L(\vec{\mathbf{x}},\vec{\mathbf{u}}) + \vec{\psi} \cdot \vec{\mathbf{F}}(\vec{\mathbf{x}},\vec{\mathbf{u}}), \qquad (3.5)$$

where L is given in Eq. (3.4) and  $\vec{F}$  is (3.1). The vector function  $\vec{\psi}(t)$  is called the *costate variable* or the *adjoint variable*. It plays a role similar to that played by Lagrange multipliers in variational calculus, it ensures that the constraint equations Eq. (3.1) are satisfied. It differs from ordinary Lagrange multipliers in that it satisfies an equation of motion:

$$\dot{\overline{\psi}}(t) = -\frac{\partial H}{\partial \dot{\overline{\mathbf{x}}}} [\dot{\overline{\mathbf{x}}}(t), \ddot{\overline{\mathbf{u}}}(t), \ddot{\overline{\psi}}(t)], \qquad (3.6)$$

where  $(\partial H/\partial \mathbf{x})_j \equiv \partial H/\partial x_j$ . It is clear why *H* is called the Hamiltonian if one notes that Eq. (3.1) may be written as

$$\dot{\mathbf{x}}(t) = \frac{\partial H}{\partial \dot{\boldsymbol{\psi}}} [\dot{\mathbf{x}}(t), \ddot{\mathbf{u}}(t), \dot{\boldsymbol{\psi}}(t)].$$
(3.7)

The Pontryagin maximum principle states that if  $\vec{u}^*(t)$  is an admissible control and  $\vec{x}^*(t)$  is the trajectory corresponding to  $\vec{u}^*$  which satisfies the boundary conditions  $\vec{x}^*(t_0) = \vec{x}_0$  and  $\vec{x}^*(t_1) = \vec{x}_1$  then if  $\vec{u}^*(t)$  is an optimal control it is necessary that  $\vec{x}^*(t)$  and  $\vec{\psi}^*(t)$  satisfy the canonical system of equations

$$\dot{\vec{\mathbf{x}}}^*(t) = \frac{\partial H}{\partial \vec{\psi}} [\vec{\mathbf{x}}^*(t), \vec{\mathbf{u}}^*(t), \vec{\psi}^*(t)], \qquad (3.8)$$

$$\dot{\overline{\psi}}^{*}(t) = -\frac{\partial H}{\partial \dot{\overline{\mathbf{x}}}} [\vec{\mathbf{x}}^{*}(t), \vec{\mathbf{u}}^{*}(t), \vec{\overline{\psi}}^{*}(t)], \qquad (3.9)$$

with  $\vec{\mathbf{x}}^*(t_0) = \vec{\mathbf{x}}_0$  and  $\vec{\mathbf{x}}^*(t_1) = \vec{\mathbf{x}}_1$ . Furthermore, the function  $H[\vec{\mathbf{x}}^*(t), \vec{\mathbf{u}}^*(t), \vec{\psi}^*(t)]$  is an absolute maximum over the set of admissible controls for t in  $[t_0, t_1]$ ; i.e.,

$$H[\vec{\mathbf{x}}^{*}(t), \vec{\mathbf{u}}^{*}(t), \vec{\psi}^{*}(t)] \ge H[\vec{\mathbf{x}}^{*}(t), \vec{\mathbf{u}}, \vec{\psi}^{*}(t)]$$
(3.10)

for any admissible u. Finally

$$H^* = H[\vec{x}^*(t), \vec{u}^*(t), \vec{\psi}^*(t)]$$
(3.11)

is a constant (for autonomous systems).

Equation (3.8)-(3.11) will provide us with the equations we need to solve our problem; however, as we shall see there are cases in which Eq. (3.10) does not place any restriction on some control variables, this case leads to what is called the singular-control problem. In our case this will not be difficult to deal with, although in general it

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is. Equation (3.11) will be recognized as the conservation of energy for dynamical systems which are invariant with respect to time translation. In fact the generalization of Eq. (3.11) to nonautonomous systems is  $dH/dt = \partial H/\partial t$ .

The Pontryagin maximum principle provides necessary conditions for solutions to the optimalcontrol problem. Sufficient conditions are more difficult to obtain and to use. However, if a unique solution to Eqs. (3.8) and (3.9) satisfying the boundary conditions (3.10) and (3.11) exists, then it is obviously the optimal solution.

#### D. Properties of the solutions to optimal-control problems

There are some properties of optimal solutions that we shall make use of in solving our problem which we wish to state now. First note that, from the general theory of ordinary differential equations, since  $\overline{u}(t)$  is piecewise continuous,  $\overline{x}(t)$  and  $\overline{\psi}(t)$  are continuous because they are solutions to Eqs. (3.8) and (3.9).

Secondly, we will make use of the *principle of* optimality which states that any portion of an optimal trajectory is also an optimal trajectory. In order to see what this means, suppose  $\vec{x}^*(t)$  is an optimal trajectory starting at  $\vec{x}^*(t_0) = \vec{x}_0$  and ending at  $\vec{x}^*(t_1) = \vec{x}_1$ , and  $\vec{u}^*(t)$  is the optimal control on  $[t_0, t_1]$  corresponding to that trajectory. Now suppose we seek an optimal trajectory  $\hat{x}^*(t)$  on the interval  $[\hat{t}_0, t_1]$  where  $t_0 < \hat{t}_0 < t_1$  such that  $\hat{x}^*(\hat{t}_0) = \vec{x}(\hat{t}_0)$ and  $\vec{x}^*(t_1) = \vec{x}_1$ . Then the principle of optimality tells us that  $\vec{x}^*(t) = \vec{x}^*(t)$  is an optimal trajectory trajectory and  $\vec{u}^*(t) = \vec{u}^*(t)$  is an optimal control.

This concludes our brief outline of the part of optimal-control theory we will need subsequently with the one exception of the singular problem already mentioned. We shall treat this problem when it arises.

## IV. OPTIMAL PERFORMANCE OF A CLASS OF ENDOREVERSIBLE ENGINES

In this section we apply the results of the previous section to study the model engine defined in Sec. II. We shall consider two cases specified by the performance goals used in Ref. 1: case (A) the average power output is a maximum and case (B) the efficiency is a maximum. We have included only those details of the calculation which may be unfamiliar to most readers.

## A. Maximum average power output

Since the period of the engine  $\tau$  is a constant maximizing the average power output in the same as maximizing Eq. (2.7). We begin by forming the

Hamiltonian from Eqs. (2.7), (2.4), and (2.5):

$$l = cT + \psi_1 F_1 + \psi_2 F_2, \tag{4.1}$$

where  $F_1$  and  $F_2$  are defined by Eqs. (3.2) and (3.3). We have used  $W/C_V$  as the performance index. It is convenient to rewrite Eq. (4.1) as

$$H = [(1 - \psi_1)T + \psi_2]c + \psi_1 \hat{\rho}(T_R - T).$$
(4.2)

The equations for the costate variables are

$$\dot{\psi}_1 = -\frac{\partial H}{\partial T} = -c(1-\psi_1) + \hat{\rho}\psi_1, \qquad (4.3)$$

$$\dot{\psi}_2 = -\frac{\partial H}{\partial \beta} = 0. \tag{4.4}$$

The canonical equations, Eqs. (2.4), (2.6), (4.3), and (4.4), are linear in the state and costate variables and may be easily solved once the control variables are specified as functions of time; however, in general these variables are determined as functions of the state and costate variables so that the canonical equations are nonlinear. Fortunately, in our case, the canonical equations will either be linear or, when they are nonlinear, easy to solve.

### 1. Application of the maximum principle

We now wish to exploit Eq. (3.10). We define

$$\Delta H = H[\vec{x}^{*}(t), \vec{u}^{*}(t), \vec{\psi}^{*}(t)] - H[\vec{x}^{*}(t), \vec{u}, \psi^{*}(t)], \quad (4.5)$$

where  $\vec{u}$  is an admissible solution. For a maximum we require that  $\Delta H \ge 0$  so

$$\Delta H = [(1 - \psi_1^*)T^* + \psi_2^*][c^* - c]$$

$$+\psi^*_{R}[\hat{\rho}^*(T^*_{R}-T^*)-\hat{\rho}(T_{R}-T^*)] \ge 0, \qquad (4.6)$$

where

$$0 \le \hat{\rho} \le \rho_0 / C_V \equiv \hat{\rho}_0, \tag{4.7}$$

$$T_L \le T_R \le T_H, \tag{4.8}$$

and

$$-c_m \le c \le c_M. \tag{4.9}$$

We now consider various possible cases separately. These will provide us with optimal solutions from which the optimum cycle will be constructed. First suppose  $\hat{\rho} = \hat{\rho}^*$  and  $T_R = T_R^*$ , then the second term in (4.6) vanishes and  $\Delta H \ge 0$  requires that

$$c^{*} = \begin{cases} c_{M} & \text{if } (1 - \psi_{1}^{*})T^{*} + \psi_{2}^{*} > 0 \\ -c_{m} & \text{if } (1 - \psi_{1}^{*})T^{*} + \psi_{2}^{*} < 0 \\ \text{undetermined if } (1 - \psi_{1}^{*})T^{*} + \psi_{2}^{*} = 0. \end{cases}$$
(4.10)

The last possibility corresponds to the singularcontrol case mentioned in Sec. III. In our case, as we shall see, it is not difficult to show that along the singular part of the trajectory  $c^*$  is constant.

Next suppose  $c = c^*$  and  $T_R = T_R^*$ , then Eq. (4.6) reduces to

$$\Delta H = \psi_1^* (T_R^* - T^*) (\hat{\rho}^* - \hat{\rho}) \ge 0$$

which implies that

$$\hat{\rho}^* = \begin{cases} \hat{\rho}_0 & \text{if } \psi_1^*(T_R^* - T^*) > 0\\ 0 & \text{if } \psi_1^*(T_R^* - T^*) < 0\\ \text{undetermined if } \psi_1^*(T_R^* - T^*) = 0. \end{cases}$$
(4.11)

The last case again corresponds to a singularcontrol problem. It is a simple matter to eliminate this case. First if  $\psi_1^*$  equals zero for a finite time interval, then in this interval  $\psi_1^* = 0$ . From Eq. (4.4) it follows that  $c^* = 0$  but this in turn implies that  $H^* = 0$ ; however, we shall see that there is an optimum solution with  $H^* > 0$  so, since  $H^*$  is constant, we cannot have  $\psi_1^* = 0$  for a finite time interval. Next suppose  $T_R^* = T^* = 0$  for a finite time interval, then  $c = c_M$  or  $-c_m$  since otherwise  $H^* = 0$ again. In this time interval we can now show that  $\hat{\rho}\psi_1^*T^*=0$  by differentiating  $H^*$  with respect to time  $(H^*=0, \text{ remember})$  and using the canonical equations to eliminate  $\dot{T}$  and  $\dot{\psi}_1$ . We have already seen that  $\psi_1^*$  cannot vanish over a finite interval and since  $T^* = T_R^* \ge T_L$  the only possibility is  $\hat{\rho}^* = 0$  so we can include this case in (4.11).

Finally, let  $c = c^*$  and  $\hat{\rho} = \hat{\rho}^*$ , Eq. (4.6) now becomes

 $\Delta H = \psi_1^* \hat{\rho}^* (T_R^* - T^*) > 0$ 

so that

$$T_{R}^{*} = \begin{cases} T_{H} & \text{if } \psi_{1}^{*} > 0 \\ T_{L} & \text{if } \psi_{1}^{*} < 0 \end{cases}$$
(4.12)

since  $\hat{\rho}^*$  is non-negative. We have already shown that the singular case  $\psi_1^* = 0$  is excluded. If  $\hat{\rho}^* = 0$ ,  $\Delta H = 0$ , the reservoir temperature is irrelevant in this case because the reservoirs uncouple from the engine.

## 2. Optimal solutions

We can now summarize the possible optimal controls and trajectories. The trajectories are obtained by solving the canonical equations for the given controls. For convenience we now drop the \* and take all subsequent functions to be optimal.

1. 
$$\hat{\rho} = 0, c = c_M \text{ or } - c_m$$
:  
 $T(t) = T(t_0)e^{-c(t-t_0)}, \quad \beta(t) = \beta(t_0) + c(t-t_0),$   
 $\psi_1(t) = 1 - [1 - \psi_1(t_0)]e^{c(t-t_0)}, \quad \psi_2(t) = \text{const.}$  (4.13)

$$H = \{ [1 - \psi_1(t)]T + \psi_2 \} c$$
  
=  $\{ [1 - \psi_1(t_0)]T(t_0) + \psi_2 \} c.$  (4.14)

H is a constant as required and the value of c is determined by Eq. (4.10).

2. 
$$\hat{\rho} = \hat{\rho}_0, T_R = T_H \text{ or } T_L, c = c_M \text{ or } -c_m$$
:  
 $T(t) = (\hat{\rho}_0/\alpha)T_R + [T(t_0) - (\hat{\rho}_0/\alpha)T_R]e^{-\alpha (t-t_0)},$   
 $\beta(t) = c(t_0) + c(t-t_0),$   
 $\psi_1(t) = c/\alpha + [\psi_1(t_0) - c/\alpha]e^{\alpha (t-t_0)},$   
 $\psi_2(t) = \text{const},$ 
(4.15)

where  $\alpha = c + \hat{\rho}_0$ . The value of c is determined by Eq. (4.10) and the value of  $T_R$  by Eq. (4.12).

3. 
$$\hat{\rho} = \hat{\rho}_0, T_R = T_H \text{ or } T_L, (1 - \psi_1)T + \psi_2 = 0;$$
  
 $T(t) = T_r, \quad \beta(t) = \beta(t_0) + c_r(t - t_0),$   
 $c_r(t) = \hat{\rho}_0(T_R/T_r - 1),$   
 $\psi_1(t) = 1 - (T_r/T_R), \quad \psi_2(t) = -T_r^2/T_R,$ 
(4.16)

where  $T_r$  is a constant. This case is the singular case which we have not yet analyzed. By differenting  $(1 - \psi_1)T + \psi_2 = 0$  on this interval and using the canonical equations to eliminate the time derivatives it is easy to show that T,  $\psi_1$ , and c must all be constant.

We have used a subscript r to correspond to the R in  $T_R$ , i.e., if  $T_R = T_H$ , r = h and if  $T_R = T_L$ , r = l. Equation (4.12) determines the value of  $T_R$  and we see from (4.16) that if  $T_R = T_H$ ,  $\psi_{1h} > 0$  implies  $T_H > T_h$  and if  $T_R = T_L$ ,  $\psi_{1l} < 0$  implies  $T_L < T_l$ . These in turn imply that  $c_h > 0$  and  $c_l < 0$ . It is easy to show that

$$H = \hat{\rho}_0 (T_R - T_r)^2 / T_r \tag{4.17}$$

which is positive. Finally we note that  $\psi_2$ , which is constant throughout the cycle, is negative if condition 3 contributes to the solution.

As we shall see both isothermal branches are part of the optimal trajectory. From this and the constancy of  $\psi_2$  and H we get

$$T_{h} = \frac{1}{2} \sqrt{T_{H}} \left( \sqrt{T_{H}} + \sqrt{T_{L}} \right), \tag{4.18}$$

$$T_{l} = \frac{1}{2} \sqrt{T_{L}} \left( \sqrt{T_{H}} + \sqrt{T_{L}} \right).$$
 (4.19)

TABLE I. Switchings.

	1	2	3	
1	a	b	a	
2	b	b or c	с	
3	a	С	a	

<sup>a</sup> Forbidden switchings.

<sup>b</sup> Allowed switching:  $\Delta c = 0$  and  $\psi_1 = 0$ .

<sup>c</sup> Allowed switching:  $\Delta T_R = 0$ ,  $(1 - \psi_1)T + \psi_2 = 0$ .

Note that as in Ref. 1, we get  $T_l/T_h = (T_L/T_H)^{1/2}$ .

There are actually eight distinct optimal solutions which we will label  $1^{\pm}$ ,  $2_{H}^{\pm}$ ,  $2_{L}^{\pm}$ ,  $3_{H}$ , and  $3_{L}$ where plus refers to  $c = c_{M}$ , minus to  $c = -c_{m}$  and H and L to the subscript on the reservoir temperature,  $T_{R}$ .

In order to determine the actual optimal trajectory, we next examine what the constancy H and the continuity of the state and costate variables imply about switchings between pairs of the optimal solutions.

## 3. Switchings

In the literature of optimal-control theory, the surfaces in state variable phase space across which optimal-control variables change discontinuously are called switching surfaces. The switchings are summarized in Table I.

First we observe that a switch between 1 and 3 is not allowed. The reason for this is that  $(1 - \psi_1)T + \psi_2$  is continuous and vanishes for case 3, but Eq. (4.14) would require that *H* approach zero as *t* approaches the switching time from the side on which case (a) holds.

A switching between cases 1 and 2 is allowed at



FIG. 1. State variables for case A, maximum power output: T is the temperature and  $\beta$  is proportional to the volume of the cylinder.



FIG. 2. Optimal controls for maximum power output:  $\rho T$  is the reservoir temperature times the thermal conductance and c is proportional to the time derivative of the logarithm of the volume of the cylinder.



FIG. 3. Costate variables for maximum power output:  $\psi_1$  is the temperature costate variable and  $\psi_2$  is the  $\beta$  costate variable.

a time when  $\psi_1$  vanishes. This can be seen by comparing Eqs. (4.14) and (4.2). Note that  $\psi_1$  may vanish at a point of time but, as we have seen above, not along an interval of time. During such a switching c must not change since  $H \neq 0$ .

A switching between cases 2 and 3 is allowed at an instant when  $(1 - \psi_1)T + \psi_2$  vanishes.  $T_R$  must remain constant during this transition since a change in  $T_R$  requires  $\psi_1 = 0$  at the instant of switching. But for case 2,  $\psi_1 \neq 0$  so by continuity such a switching is eliminated.

Next observe that there cannot be a switching between 1<sup>\*</sup> and 1<sup>-</sup>, since at such a transition Eq. (4.10) requires that  $(1 - \psi_1)T + \psi_2$  vanish but then (4.14) leads to H = 0. We also cannot have a switching between  $3_H$  and  $3_L$  because of the continuity of  $\psi_1$ . It is, however, possible to have a switching in case 2 between  $T_R = T_H$  and  $T_R = T_L$  with c remaining constant provided  $\psi_1$  passes through zero at the switching time. It is also possible for a switching between  $-c_m$  and  $c_M$  to occur with  $T_R$  unchanged provided  $(1 - \psi_1)T + \psi_2$  vanish at the switching. However, both  $T_R$  and c cannot change simultaneously since this requires that H = 0.

One interesting and surprising observation is that a switching between an isothermal and adiabatic is not allowed along an optimal trajectory. In fact it turns out that the optimal trajectory has no adiabatic branches.

#### 4. Optimal controls and trajectory

After this rather lengthy discussion of the possible optimal subtrajectories we are ready to work out the optimal cycle. As explained at the end of Sec. IV, the principle of optimality implies that the cases discussed above may be smoothly connected to construct the optimal trajectory. Furthermore since our system is autonomous, i.e., invariant with respect to time translation, we may choose any point along our optimal trajectory as a starting point.

Figures 1-3 summarize the behavior of the state, control, and costate variables along the trajectory. We will begin by assuming that we are at the beginning of a  $3_H$  branch, i.e.,  $T_R = T_H$ ,  $T = T_h$ , etc. for  $0 \le t \le t_1$ . The only allowed switching is to a branch  $2_H^+$ , i.e.,  $T_R = T_H$ ,  $c = c_M$ , etc. For t between  $t_1$  and  $t_2$ ,  $\psi_1$  decreases and  $T(1 - \psi_1) + \psi_2$  increases from zero—as it must if  $c = c_M$ . Thus the only possible transition occurs at  $t_2$  when  $\psi_1$  vanishes and we get a  $2_L^*$  branch. It would be possible to have a transition to the adiabat 1<sup>\*</sup>, however, it turns out that this does not occur. To show this it is necessary to include such a branch and show that the optimal solution leads to the branch occuring for zero time. We shall see in Sec. IV B that an adiabatic branch does occur when we maximize efficiency and the branch drops out of the solution in the limit that corresponds to the maximum power output.

From  $t_2$  to  $t_3$ ,  $\psi_1$  continues to decrease and so does  $T(1-\psi_1)+\psi_2$  until it vanishes at which time another switch becomes possible. At  $t_3$  we begin an isothermal branch  $3_L$  which lasts until the time  $t_4$  when we switch to a  $2_L$  branch. Along this branch  $T(1-\psi_1)+\psi_2$  decreases from zero while  $\psi_1$ increases until it reaches zero at  $t_5$ . At this time we switch to a  $2_H$  branch until  $T(1-\psi_1)+\psi_2$  returns to zero at the end of the cycle  $t_6=\tau$ . Again it is possible for an adiabat to occur between the branches  $2_L^2$  and  $2_H^2$  but again this is not part of the optimal trajectory.

So far we have not explained how the times  $t_1$ through  $t_6$  are calculated.  $t_2 - t_1$  and  $t_5 - t_4$  are determined by the vanishing of  $\psi_1$  while  $t_3 - t_2$  and  $t_6 - t_5$  are determined by the vanishing of  $T(1 - \psi_1)$  $+ \psi_2$ .  $t_1$  and  $t_4 - t_3$  are then fixed by the length of the cycle, i.e.,  $t_6 = \tau$ , and by the end conditions on  $\beta$ , i.e.,  $\beta(0) = \beta(\tau) = 0$  taking  $V_0$  to be the smallest value of the volume. Once  $t_2 - t_2$  and  $t_5 - t_4$  are determined,  $T(t_2)$  and  $T(t_3)$  are determined.

The complete solution may now be recorded. It is convenient to define the quantities

$$x = (T_L/T_H)^{1/2},$$
  

$$\alpha_* = c_M + \hat{\rho}_0, \quad \alpha_- = c_m - \hat{\rho}_0,$$
  

$$\epsilon_M = \hat{\rho}_0/c_M, \quad \epsilon_m = \hat{\rho}_0/c_m.$$
(4.20)

Since  $\psi_2$  is constant throughout the cycle we record it only once. Then from (4.16) and (4.19) we have the following:

$$T = \frac{1}{2}T_H(1+x), \quad \beta = c_h t;$$
  

$$T_R = T_H, \quad c = c_h = \hat{\rho}_0(1-x)/(1+x);$$
  

$$\psi_1 = \frac{1}{2}(1-x), \quad \psi_2 = -\frac{1}{4}T_H(1+x)^2.$$

For  $t_1 \leq t \leq t_2$ 

for  $0 \le t \le t_1$ 

$$T = T_H \left[ \frac{\epsilon_M}{1 + \epsilon_M} \left( \frac{1}{2} (1 + x) - \frac{\epsilon_M}{1 + \epsilon_M} \right) e^{-\alpha_+ (t - t_1)} \right]$$
  
$$\beta = c_M (t - t_1) + c_h t_1,$$
  
$$T_R = T_H, \quad c = c_M,$$
  
$$\psi_1 = \frac{1}{1 + \epsilon_M} - \left( \frac{1}{2} (1 + x) - \frac{\epsilon_M}{1 + \epsilon_M} \right) e^{\alpha_+ (t - t_1)}.$$

For  $t_2 \leq t \leq t_3$  $T = T_L \left[ \frac{\epsilon_M}{1 + \epsilon_M} + \left( \frac{T_2}{T_L} - \frac{\epsilon_M}{1 + \epsilon_M} \right) e^{-\alpha_+(t - t_2)} \right],$   $\beta = c_M(t - t_1) + c_h t_1,$   $T_R = T_L, \quad c = c_M,$   $\psi_1 = \left[ 1/(1 + \epsilon_M) \right] (1 - e^{\alpha_+(t - t_2)}),$   $T_2 = \frac{1}{4} T_H \left[ (1 + x)^2 + \epsilon_M (1 - x)^2 \right].$ 

For  $t_3 \leq t \leq t_4$ 

$$T = \frac{1}{2}T_{L}[(1/x) + 1],$$
  

$$\beta = c_{I}(t - t_{3}) + c_{m}(t_{3} - t_{1}) + c_{h}t_{1},$$
  

$$T_{R} = T_{L}, \quad c = c_{I} = -c_{h},$$
  

$$\psi_{1} = -\frac{1}{2}[(1/x) - 1].$$

For  $t_4 \leq t \leq t_5$ 

$$T = T_L \left\{ -\frac{\epsilon_m}{1-\epsilon_m} + \left[ \frac{1}{2} \left( \frac{1}{x} + 1 \right) + \frac{\epsilon_m}{1-\epsilon_m} \right] e^{\alpha_-(t-t_d)} \right\},$$
  
$$\beta = -c_m(t-t_d) + c_1(t_d-t_3) + c_M(t_3-t_1) + c_h t_1,$$
  
$$T_R = T_L, \quad c = -c_m,$$
  
$$\psi_1 = \frac{1}{1-\epsilon_m} \left[ \frac{1}{2} \left( \frac{1}{x} + 1 \right) + \frac{\epsilon_m}{1-\epsilon_m} \right] e^{-\alpha_-(t-t_d)}.$$

For  $t_5 \leq t \leq t_6 = \tau$ 

$$\begin{split} T &= T_{H} \left[ \frac{\epsilon_{m}}{1 - \epsilon_{m}} + \left( \frac{T_{5}}{T_{H}} + \frac{\epsilon_{m}}{1 - \epsilon_{m}} \right) e^{\alpha_{-}(t - t_{5})} \right], \\ \beta &= -c_{m}(t - t_{4}) + c_{1}(t_{4} - t_{5}) + c_{M}(t_{3} - t_{1}) + c_{h}t_{1}, \\ T_{R} &= T_{H}, \quad c = -c_{m}, \\ \psi_{1} &= \frac{1}{1 - \epsilon_{m}} (1 - e^{-\alpha_{-}(t - t_{5})}), \end{split}$$

$$T_5 = \frac{1}{4}T_H [(1+x)^2 - \epsilon_m (1-x)^2].$$

As we stated above  $t_2 - t_1$  and  $t_5 - t_4$  are determined by  $\psi_1 = 0$  so we find

$$t_2 - t_1 = -\frac{1}{\alpha_+} \ln\left(\frac{1+x}{2} - \epsilon_M \frac{1-x}{2}\right)$$

and

$$t_5 - t_4 = +\frac{1}{\alpha_-} \ln \left[ \frac{1}{2} \left( \frac{1}{x} + 1 \right) - \epsilon_m \frac{1}{2} \left( \frac{1}{x} - 1 \right) \right].$$

To determine  $t_3 - t_2$  and  $t_6 - t_5$  we use the vanishing  $T(1 - \psi_1) + \psi_2$  at  $t_3$  and  $t_6$  and we find

$$t_3 - t_2 = \frac{1}{\alpha_*} \ln \left[ \frac{1}{2} \left( \frac{1}{x} + 1 \right) + \epsilon_M \frac{1}{2} \left( \frac{1}{x} - 1 \right) \right]$$

and

$$t_6 - t_5 = -\frac{1}{\alpha} \ln[\frac{1}{2}(1+x) + \epsilon_m \frac{1}{2}(1-x)].$$

These are positive provided  $\epsilon_m$  and  $\epsilon_M$  are both less than 1. For physically reasonable systems these quantities will generally be much less than 1 since they are the ratio of adiabatic relaxation time  $(1/c_m \text{ or } 1/c_M)$  to the heat-conduction time constant  $(1/\hat{\rho}_0)$ .

Finally we can determine  $t_1$  and  $t_4 - t_3$  since

$$t_1 + (t_4 - t_3) = \tau - (t_3 - t_1) - (t_6 - t_5)$$

and from  $\beta(t_6) = 0$ 

$$c_{h}[t_{1}-(t_{4}-t_{3})]=-c_{M}(t_{3}-t_{1})+c_{m}(t_{6}-t_{4}),$$

we get

$$t_{1} = \frac{\tau}{2} - \left(1 + \frac{c_{M}}{c_{h}}\right)(t_{3} - t_{1}) - \left(1 - \frac{c_{m}}{c_{h}}\right)(t_{6} - t_{4}),$$
  
$$t_{4} - t_{3} = \frac{\tau}{2} - \left(1 - \frac{c_{M}}{c_{h}}\right)(t_{3} - t_{1}) - \left(1 + \frac{c_{m}}{c_{h}}\right)(t_{6} - t_{4}).$$

Of course these must be positive numbers. This means that if we had taken  $\tau$  too small there would not be any solution to our problem.

In general no two of the time intervals are equal even if  $c_M = c_m$ . However, if  $\epsilon_M$  and  $\epsilon_m$  are both much less than 1 it is easy to show that  $t_1$  and  $(t_4 - t_3)$  are equal to  $\frac{1}{2}\tau[1 + O(1/c\tau)]$  where c is either  $c_m$  or  $c_M$  and the other four time intervals are of order  $\tau(1/c\tau)$ .

It is now a simple matter to work out W and  $Q_1$  using Eqs. (2.7) and (2.8).

$$\begin{split} W &= C_V \hat{\rho}_0 \bigg[ \frac{1}{2} (\sqrt{T_H} - \sqrt{T_L}) [\sqrt{T_H} t_1 - \sqrt{T_L} (t_4 - t_3)] \\ &+ \frac{C_M}{\alpha_+} [T_H (t_2 - t_1) + T_L (t_3 - t_2)] \\ &+ \frac{C_m}{\alpha_-} [T_L (t_5 - t_4) + T_H (t_6 - t_5)] \\ &- \left(\frac{1}{\alpha_+} + \frac{1}{\alpha_-}\right) \left(\frac{T_H - T_L}{2}\right) \bigg] , \\ Q_1 &= C_V \hat{\rho}_0 \bigg[ \frac{1}{2} \sqrt{T_H} (\sqrt{T_H} - \sqrt{T_L}) t_1 \\ &+ T_H \bigg( \frac{C_M}{\alpha_+} (t_2 - t_1) + \frac{C_m}{\alpha_-} (t_6 - t_5) \bigg) \\ &- \frac{1}{\alpha_+} [\frac{1}{4} (T_H - T_L) - \frac{1}{4} \epsilon_M (\sqrt{T_H} - \sqrt{T_L})^2] \bigg] \\ &- \frac{1}{\alpha_-} [\frac{1}{4} (T_H - T_L) + \frac{1}{4} \epsilon_m (\sqrt{T_H} - \sqrt{T_L})^2] \bigg] \end{split}$$

In the limit that  $\epsilon_m$  and  $\epsilon_M$  become small compared to 1, the leading term in each of these expressions is the same as found in Ref. 1. In the limit that  $\epsilon_m$ and  $\epsilon_M$  vanish, the process reduces to that of Ref. 1 with the nonisothermal branches becoming adiabatic branches which occur for vanishingly short times; i.e., the temperature T changes discontinuously.

This rather lengthy section completes our solution to the optimization problem for the performance goal of maximum power output.

# B. Maximum efficiency

We now turn to our second choice of an operational goal, maximizing the efficiency for fixed cycling time and input energy. As in Ref. 1 we must now maximize  $W - \mu Q_1$  where W and  $Q_1$  are given by Eqs. (2.7) and (2.8) and  $\mu$  is an ordinary Lagrange multiplier which is determined so that  $Q_1$  equals the given input energy.

The procedure for determing the optimal solution is identical to that in Sec. IVA. The Hamiltonian may be written in the form

$$H = [(1 - \psi_1)T + \psi_2]c + [\psi_1 - \mu \theta (T_R - T)]\hat{\rho}(T_R - T).$$
(4.21)

This reduces to the Hamiltonian in Eq. (4.2) if  $\mu = 0$ . The equations for the costate variables are easily derived.

The derivation of the optimal solution is complicated by the  $\mu$  term. In Appendix A we show that  $\mu = \partial W_{\max} / \partial Q_1$ , i.e.,  $\mu$  is a measure of the sensitivity of  $W_{\max}$  with respect to small changes in the constraint,  $Q_1 = \text{const.}$  From Fig. 1 of Ref. 1 we see that  $\mu$  can be both positive and negative and  $\mu$ vanishes for the maximum power output, as expected.

To simplify the subsequent discussion we shall assume  $\mu \ge 0$ , the results for  $\mu \le 0$  will be mentioned where appropriate.

In the following we will limit our discussion to the changes in the analysis brought about by the presence of the extra constraint. We shall see that the optimal trajectory now contains adiabatic branches between the  $2_H^{\pm}$  and  $2_L^{\pm}$  branches.

#### 1. Application of the maximum principle

As in Sec. IV A, we begin with Eqs. (4.5) and (4.6). The second term in Eq. (4.6) is different in the present case because of the  $\mu$  term in Eq. (4.21); however, this does not effect the analysis leading to the results (4.10).

Equation (4.11) is changed, we now find, setting  $c = c^*$  and  $T_R = T_R^*$ , that  $\Delta H \ge 0$  requires

$$\hat{\rho}^{*} = \begin{cases} \hat{\rho}_{0} & \text{if } [\psi_{1}^{*} - \mu^{*}\theta(T_{k}^{*} - T^{*})](T_{k}^{*} - T^{*}) > 0, \\ 0 & \text{if } [\psi_{1}^{*} - \mu^{*}\theta(T_{k}^{*} - T^{*})](T_{k}^{*} - T^{*}) < 0, \\ \text{undetermined if } [\psi_{1}^{*} - \mu^{*}\theta(T_{k}^{*} - T^{*})] \\ (T_{k}^{*} - T^{*}) = 0. \end{cases}$$

The last possibility is the singular case. It can be eliminated as a possibility because it leads to the requirement  $\psi_1 = \mu = 1$  which would in turn lead to  $H^* = 0$  but we shall see, as in Sec. IV A,  $H^* > 0$ . Finally, let  $c = c^*$  and  $\hat{\rho} = \hat{\rho}^*$ ,

 $\Delta H = \begin{cases} \hat{\rho}^* \{ \psi_1^*(T_R^* - T_R) \\ -\mu^* [T_R^* - T^* - \theta(T_R - T^*)(T_R - T^*)] \} \\ & \text{if } T_R^* > T^* \\ \hat{\rho}^* \{ \psi_1^*(T_R^* - T_R) \\ +\mu^* \theta(T_R - T^*)(T_R - T^*) \} \text{ if } T_R^* \leq T^*. \end{cases}$ 

From (4.22)  $\hat{\rho}^* = \hat{\rho}_0$  requires  $\psi_1^* > \mu^*$  if  $T_R^* > T^*$  and  $\psi_1^* < 0$  if  $T_R^* < T^*$ . By first considering  $T_R$  in the interval  $[T^*, T_H]$  for  $T_R^* > T^*$  we find  $T_R^* = T_H$  in order that  $\Delta H \ge 0$ . It then follows that  $\Delta H \ge 0$  for  $T_R^*$  in the interval  $[T_L, T^*]$  since  $\mu^* \ge 0$ . In a similar fashion, when  $T_R^* < T^*$ ,  $\Delta H \ge 0$  provided  $T_R^* = T_L$ . Thus in place of Eq. (4.12) we have

$$T_{R}^{*} = \begin{cases} T_{H}, & \psi_{1}^{*} > \mu^{*} \\ T_{L}, & \psi_{1}^{*} < 0 \end{cases}$$
(4.24)

and for  $\hat{\rho}^* \neq 0$ ,  $T_H > T^* > T_L$ .

This result is different from the similar result in Sec. IV A because we cannot directly switch from the high- to the low-temperature reservoir if  $\mu > 0$ . We shall see that this introduces an adiabatic branch in the optimal solution. If  $\mu^* \le 0$  the adiabatic branch may be dispensed with—as we saw for  $\mu^* = 0$ . For  $\mu \le 0$  a more complicated result replaces (4.24).

#### 2. Optimal solutions

We now summarize the possible optimal controls and trajectories. As we did in Sec. IV A, we drop the \* and take all subsequent expressions to be optimal.

Case 1 is identical to that given in (4.13).

2. 
$$\hat{\rho} = \hat{\rho}_0$$
,  $T_R = T_H$  or  $T_L$ ,  $c = c_M$  or  $-c_m$ :  
 $T(t) = \frac{\hat{\rho}_0}{\alpha} T_R + \left( T(t_0) - \frac{\hat{\rho}_0}{\alpha} T_R \right) e^{-\alpha (t-t_0)}$ ,  
 $\beta(t) = \beta(t_0) + c(t-t_0)$ ,  
 $\psi_1(t) = \frac{c}{\alpha} + \frac{\hat{\rho}_0}{\alpha} \mu \theta(T_R - T)$   
 $+ \left( \psi_1(t_0) - \frac{c}{\alpha} - \frac{\hat{\rho}_0}{\alpha} \mu \theta(T_R - T) \right) e^{\alpha (t-t_0)}$ ,  
 $\psi_2(t) = \text{const}$ , (4.25)

where  $\alpha = c + \hat{\rho}_0$  and the values of c and  $T_R$  are determined by Eqs. (4.10) and (4.24), respectively.

 $\psi_1(t) = 1 - (T_r/T_R)A_R, \quad \psi_2(t) = - (T_r^2/T_R)A_R$  (4.26)

where  $T_r$  is a constant and we have used the same notation as in Sec. IVA where r = h when R = Hand r = l when R = L. The only difference between these solutions and those of (4.16) arises from the presence of  $A_R$ ,

$$A_{R} = \begin{cases} 1 - \mu, & R = H \\ 1, & R = L. \end{cases}$$
(4.27)

We also see that  $c_h$  is a positive constant and  $c_t$  is a negative constant just as in Sec. IVA. From  $\psi_{1h} > \mu$  it follows that  $\mu < 1$  and, finally, it is easy to show that

$$H = \hat{\rho}_0 A_r (T_R - T_r)^2 / T_R \tag{4.28}$$

which may be compared with Eq. (4.17).

Since both branches occur in the optimal cycle, the constancy of H and  $\psi_2$  imply that

$$T_{H} = \frac{1}{2} \left( \frac{T_{H}}{(1-\mu)} \right)^{1/2} \{ [T_{H}(1-\mu)]^{1/2} + \sqrt{T_{L}} \},$$
  
$$T_{I} = \frac{1}{2} \sqrt{T_{L}} \{ [T_{H}(1-\mu)]^{1/2} + \sqrt{T_{L}} \},$$
 (4.29)

which reduces to (4.19) when  $\mu = 0$ .

Thus once again we have eight possibilities from which to select the pieces of the optimal cycle.

#### 3. Switchings

The switchings are summarized in Table II. The switchings are different from those shown in Table I. For example, the choice of R in a switch from  $1^+$  to  $2_R^+$  was determined in Sec. IV A by whether  $\psi_1$  was increasing or decreasing through zero. In the case under study in this section a switching from  $1^+$  to  $2_H^+$  requires that  $\psi_1$  rise through  $\mu$  while in a switching from  $1^+$  to  $2_H^+$  requires that  $\psi_1$  fall through zero.

TABLE II. Switchings.

	1	2	3
1	a	b or c	a
2	b or c	d	d
3	a	d	a

<sup>a</sup> Forbidden switching.

<sup>b</sup>Allowed switching:  $\Delta c = 0$  and  $\psi_1 = 0$ .

<sup>c</sup> Allowed switching:  $\Delta c = 0$  and  $\psi_1 = \mu$ .

<sup>d</sup>Allowed switching:  $\Delta T_R = 0$ ,  $(1 - \psi_1)T + \psi_2 = 0$ .



FIG. 4. State variables for case B, maximum efficien-  $\operatorname{cy.}$ 



FIG. 5. Optimal controls for maximum efficiency.



FIG. 6. Costate variables for maximum efficiency.

Similarly where in Sec. IV A a switching between  $2_H^*$  and  $2_L^*$  was allowed if  $\Delta c = 0$ , provided  $\psi_i = 0$  at the switching time, we no longer can have such a switching when  $\mu \ge 0$  because  $\psi_1$  must vary continuously. If  $\mu \le 0$ , the switching is allowed.

#### 4. Optimal controls and trajectory

Figures 4-6 summarize the optimal solution. As before we begin on  $3_H$  branch for  $0 \le t \le t_1$ . The cycle differs from that of Sec. IV A by the appearance of two adiabatic branches. The first occurs between the  $2_H^*$  and  $2_L^*$  branches and the second between  $2_L^*$  and  $2_H^*$ .

Fortunately the form of the optimal solution is similar to the form of the solution in Sec. IV A. If we replace x from (4.20) by

$$y = \left(\frac{1}{1-\mu} \frac{T_L}{T_H}\right)^{1/2}$$
(4.30)

then starting on the branch  $3_H$ , we have from (4.26).

for 
$$0 \le t \le t_1$$
  
 $T = \frac{1}{2}T_H(1+y), \quad \beta(t) = c_h t,$   
 $T_R = T_H, \quad c = c_h = \hat{\rho}_0 \frac{1-y}{1+y},$   
 $\psi_1 = 1 - \frac{1}{2}(1-\mu)(1+y), \quad \psi_2 = -\frac{1}{4}T_H(1+y)^2(1-\mu).$ 

Note that the costate variables  $1 - \psi_1$  and  $\psi_2$  are multiplied by  $1 - \mu$  in addition to having x replaced by y. Also observe that when  $\mu$  is set equal to zero we get the result of Sec. IV A back.

For  $t_1 < t \le t_2$  and  $t_5 \le t \le t_6$  the solution may be obtained from Sec. IV A by replacing x by y and  $1 - \psi_1$  by  $(1 - \mu)(1 - \psi_1)$ . Similarly for  $t'_2 < t \le t_3$ ,  $t_3 < t \le t_4$  and  $t_4 < t \le t'_5$ , the solution for Sec. IV B follows from Sec. IV A with x replaced by y, but now  $1 - \psi_1$  is not multiplied by a factor of  $1 - \mu$ . The appearance of the primed times is due to the existance of the two adiabatic branches for  $t_2 < t$  $\le t'_2$  and  $t'_5 \le t \le t_5$ . The expressions for  $T_2$  and  $T_5$ in Sec. IV A become  $T'_2$  and  $T'_5$ , respectively, when x is replaced by y. For the adiabatic branches we have the following: for  $t_2 < t \le t'_2$ 

 $+ c_{h}t_{1}$ ,

$$T(t) = T_2 e^{-c_M (t-t_2)}, \quad \beta(t) = c_M (t-t_1)$$
$$\hat{\rho}_0 = 0, \quad c = c_M,$$

$$\psi_1(t) = 1 - (1 - \mu)e^{c_M(t-t_2)}$$

where  $T_2 = T'_2/(1 - \mu)$ . For  $t'_5 < t \le t_5$ 

$$T(t) = T'_{5}e^{c_{m}(t-t_{5}^{c})}\beta(t)$$
  
=  $-c_{m}(t-t_{4}) + c_{1}(t_{4}-t_{5}) + c_{M}(t_{5}-t_{1}) + c_{h}t_{1},$   
 $\hat{p}_{0} = 0, \quad c = -c_{m},$   
 $\psi_{1}(t) = 1 - e^{-c_{m}(t-t_{5}^{c})}.$ 

The duration of all the branches except the isothermal branches is again determined by the switching conditions. For example,  $t'_2$  is determined by  $\psi_1(t'_2) = 0$ , so

$$t_2' - t_2 = -(1/c_M) \ln(1-\mu)$$

while  $t_5$  is determined by  $\psi_1(t_5) = \mu$ , so

$$t_5 - t_5' = -(1/c_m) \ln(1-\mu).$$

For these two times to be finite and positive we must have  $1 > \mu > 0$ . The remaining times can be obtained from Sec. IVA by simply replacing x by y, and  $t_2$  and  $t'_2$  and  $t_5$  by  $t'_5$  in the appropriate places. The expressions for  $t_1$  and  $t_4 - t_5$  in terms of  $\tau$ ,  $t_3 - t_1$ , and  $t_6 - t_4$  are identically the same as the corresponding expressions in Sec. IVA.

The expressions for  $Q_1$  may be obtained from Sec. IVA by simply replacing  $T_L$  by  $T_L/(1-\mu)$  and using the expressions for the times with x replaced by y. The expression for W is more complicated.

$$\begin{split} W &= C_{V} \hat{\rho}_{0} \left( \frac{1}{2} \left[ \sqrt{T_{H}} - \left( \frac{T_{L}}{1 - \mu} \right)^{1/2} \right] \left\{ \sqrt{T_{H}} t_{1} - [T_{L}(1 - \mu)]^{1/2} (t_{4} - t_{3}) \right\} \\ &+ \frac{c_{M}}{\alpha_{\star}} [T_{H}(t_{2} - t_{1}) + T_{L}(t_{3} - t_{2}')] \\ &+ \frac{c_{m}}{\alpha_{\star}} [T_{L}(t_{5}' - t_{4}) + T_{H}(t_{6} - t_{5})] + \left( \frac{1}{\alpha_{\star}} + \frac{1}{\alpha_{\star}} \right)^{\frac{1}{2}} (T_{H} - T_{L}) \\ &+ \frac{\mu}{1 - \mu} \left\{ \left( \frac{1}{\alpha_{\star}} + \frac{1}{\alpha_{\star}} \right)^{\frac{1}{4}} \left[ T_{H} + \frac{T_{L}}{1 - \mu} + 2\mu \left( \frac{T_{H}T_{L}}{1 - \mu} \right)^{1/2} \right] + \frac{1}{4} \left( \frac{1}{\alpha_{\star}} \epsilon_{m} - \frac{1}{\alpha_{\star}} \epsilon_{m} \right) \left[ \sqrt{T_{H}} - \left( \frac{T_{L}}{1 - \mu} \right)^{1/2} \right]^{2} \right\} \right) \,. \end{split}$$

To complete our calculation, it is necessary to solve for  $\mu$  in terms of  $Q_1$ . This can only be done numerically, even in the limit of small  $\epsilon_M$  and  $\epsilon_m$ , and we have not bothered to do this.

The optimal trajectory and controls reduce to those of Sec. IV A in the limit  $\mu = 0$ . For  $\mu < 0$ , the adiabatic branches do not occur. We will not discuss this case.

## V. SUMMARY AND CONCLUSIONS

We have shown in detail how to obtain optimal operating configurations for a class of irreversible heat engines. The essential feature of this work is to show how to incorporate processes which generate power into thermodynamics. To do this it has been necessary to explicitly incorporate irreversibility into our discussion. By limiting ourselves to an idealized set of engines we have succeeded in studying these processes analytically.

We wish to stress that determining reasonable standards of performance for energy conversion processes cannot rely upon reversible processes. A standard such as second-law efficiency is too idealized to use. Most power generating systems, i.e., systems that perform finite work in finite time, do not come near achieving second-law efficiency and one has no idea what the margin for improvement is. This work, along with the works mentioned in Ref. 1, hopefully will provide a first step toward a better theory of thermodynamic processes.

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#### APPENDIX A

We wish to show that  $dW_{\rm max}/dQ_1 = \mu$ , i.e., the Lagrange multiplier is a measure of the variation of  $W_{\max}$  with respect to a small change in the constraint condition that  $Q_1$  is a constant.<sup>4,7</sup>

Let

$$W_{\max}(E) = \int_0^\tau f_0(\vec{\mathbf{x}}, \vec{\mathbf{u}}) dt, \qquad (A1)$$

$$Q_1 = \int_0^{\infty} g(\vec{\mathbf{x}}, \vec{\mathbf{u}}) dt, \qquad (A2)$$

where  $\mathbf{x}$  are the state variables and  $\mathbf{u}$  are the control variables. W is maximized subject to the constraint  $Q_1 = E$  where E is a fixed positive number. The Hamiltonian is of the form

$$H = f_0 - \mu g + \psi_0 \vec{\mathbf{f}} \tag{A3}$$
 with

$$\dot{\vec{x}} = \vec{f}(\vec{x}, \vec{u}). \tag{A4}$$

We now wish to compute  $dW_{max}/dE$ . For simplicity we will assume that each component of the admissible controls can be parametrized by a variable w such that as  $w_j$  runs from  $-\infty$  to  $\infty$ ,  $u_j$  runs through its admissible values from its minimum to its maximum value.<sup>8</sup> Then for any functional y,  $\partial y / \partial w_j = (\partial y / \partial u_j) (\partial u_j / \partial w_j)$ . Then Eq. (3.10) implies that  $\partial H / \partial \vec{w} = 0$  where  $\partial H / \partial u_j = 0$  if the optimal control  $u_j$  occurs for  $u_j \in (u_{j\min}, u_{j\max})$  and  $\partial u_j / \partial u_j$  $\partial w_j = 0$  if the optimal control occurs for  $u_j = u_{j\min}$ or  $u_{j \max}$ .

$$\frac{dW_{\max}}{dE} = \int_{0}^{\tau} \left( \frac{\partial f_{0}}{\partial \mathbf{\hat{x}}} \cdot \frac{d\mathbf{\hat{x}}}{dE} + \frac{\partial f_{0}}{\partial \mathbf{\hat{w}}} \cdot \frac{d\mathbf{\hat{w}}}{dE} \right) dt.$$
(A5)

Using Eq. (A3), the canonical equations and  $\partial H/$  $\partial \mathbf{\tilde{w}} = 0$ , we find

$$\frac{dW_{\max}}{dE} = \int_0^{\tau} \left[ \mu \left( \frac{\partial g}{\partial \vec{x}} \cdot \frac{d\vec{x}}{dE} + \frac{\partial g}{\partial \vec{w}} \cdot \frac{d\vec{w}}{dE} \right) - \overleftarrow{\psi} \cdot \frac{d\vec{x}}{dE} - \overrightarrow{\psi} \cdot \frac{d\vec{t}}{dE} \right] dt.$$

The first term is just  $\mu dQ_1/dE = \mu$ . Integrating the second term by parts yields

$$\frac{dW_{\max}}{dE} = \mu - \left(\vec{\psi} \cdot \frac{\partial \vec{x}}{\partial E}\right)_0^{\tau} + \int_0^{\tau} \vec{\psi} \cdot \left(\frac{d\vec{x}}{dE} - \frac{d\vec{f}}{dE}\right) dt.$$

The second term vanishes because of periodicity and the last term vanishes because of Eq. (A4). Thus we obtain the desired result.

The result for variational calculus follows by simply dropping the equation of motion (A4).

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Hill, New York, 1966).

- <sup>7</sup>M. M. Denn, *Optimization By Variational Methods* (McGraw-Hill, New York, 1969).
- <sup>8</sup>An example of such a parametrization may be found in Ref. 1, Eq. (3.2).
- <sup>9</sup>An exception to this is B. Andresen, R. S. Berry, A. Nitzan, and P. Salamon, Phys. Rev. A <u>15</u>, 2086 (1977). In that paper, which stimulated this work, the authors recognize that optimal-control theory is the proper tool for attacking the problem of interest to us. The authors do not, however, employ the full power of the theory but limit themselves to finding the best cycling path out of a predetermined set of paths.