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Thermodynamics with time: Exergy and passivity

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Dedicated to the memory of my great friend, Jan C. Willems

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ABSTRACT

In this paper we continue the exploration started in the joint paper Brockett and Willems (1978) with a view toward the further development of models for characterizing the limits on energy flow in mixed thermal–mechanical systems. We put the thermodynamic concept of *exergy*[1] (available energy) in system theoretic terms and discuss its use as a storage function in the context of input–output models. In important cases the reachable sets for the systems considered here are not closed and of course this complicates any discussion of optimality. Only through the consideration of the closure of the reachable sets can the connection between optimal trajectories of dynamical systems and the basic results of classical thermodynamics be made tight.

1. Introduction

Over the years there has been considerable work generalizing classical thermodynamics by relaxing the usual assumptions on reversibility. One goal of such developments is to construct a theory that includes processes which are carried out in finite time. A common feature of such efforts is the identification of thermodynamic processes with trajectories of dynamical systems with control terms. Papers describing irreversible processes, such as that described in Orlov and Berry [1], often take this approach. The paper of Alonso and Ydstie [2] adopts a more classical approach in merging thermodynamics and control, adapting Willems' ideas on dissipative systems [3,4] to thermodynamic models. The widely cited paper of Kubo [5] links the work of Einstein on Brownian motion and diffusion to the work of Nyquist and Johnson on noise in electrical circuits, united under the general framework provided by the fluctuation–dissipation relationship and a suitable use of linear response theory.[2]

In the papers [6,7] it is argued that the theory of stochastic control provides a natural setting for many problems in this area, especially those involving nonequilibrium phenomena. Expressing matters in terms of stochastic differential equations, this work develops some basic thermodynamic ideas starting from linear stochastic differential equations and uses them to model thermal reservoirs, formulate a equipartition of energy theorem, etc. These papers make use of the Nyquist–Johnson [8] description of electrical noise in a resistors. The resulting equations can be used to study both transient (irreversible) and steady state (reversible) behavior. As in this earlier work, we are concerned here with modeling the behavior of systems in which thermal and mechanical effects interact. The new results contained in this paper include:

1. An identification of the role of what is here called *infinitesimal bracketing* and the nonexistence of optimal controls for significant classes of problems relating to thermal–mechanical systems.
2. A control theoretic model for the generation of mechanical work from thermal sources and a description of control policies which generate an amount of work which comes arbitrarily close to the classical bound.
3. A model for the use of exergy as a storage function for systems with mixed mechanical and thermal inputs.

2. Quasi-static paths and infinitesimal bracketing

The first law of thermodynamics is stated with no reference to time and the second law only refers to the directionality of time. At

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[1] The term exergy was coined by Zoran Rant in the 1950s. We choose to use it here instead of one of the other possible names such as available work, available energy, utilizable energy, etc. because it has a single precise meaning. Willems uses the term available energy in his major work on dissipative systems (Willems1972a, 1972b) but in a generic way.

[2] To a student of linear system theory, *linear response theory* as used by Kubo can be thought of as describing matters in terms of input–output behavior, impulse responses, correlation functions, power spectra, etc., rather than using linear differential equations as is done in [6].

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important points, classical thermodynamics is constructed around ideas relating to quasi-static processes. The relationship between the paths defined by quasi-static processes and trajectories in the sense of dynamical systems is not part of the theory. In many cases the paths followed when executing a quasi-static process are not integral curves of any clearly identified physical system and must be thought of as a particular kind of limiting form.

We discuss two quite distinct problems arising in this time-based approach to thermodynamics relating to the nonexistence of optimal trajectories. The first is that in some situations better performance can be obtained by extending the time interval indefinitely. Secondly, for some problems for which Lie bracketing plays a role, better performance can be obtained by allowing the total variation of a trajectory to approach infinity; this will be referred to here as *infinitesimal bracketing issue*.

2.1. Infinite time intervals (quasistatic processes)

Perhaps the simplest example of this is the following. Consider the scalar equation $\dot{x} = u$; $x(0) = 0$ and suppose one is to find the control u defined on the interval $[0, \infty)$ such that $x(\infty) = 1$ and the quantity

$$\eta = \int_0^\infty u^2 dt$$

is minimized. This can also be expressed as finding u such that

$$\int_0^\infty u\,dt = 1; \qquad \eta = \int_0^\infty u^2\,dt = \text{minimum}.$$

This problem has no solution because by setting $u = \epsilon$ on $[0, 1/\epsilon]$ one has $\eta = \epsilon$ and this can be made as small as we like but not zero. This will be referred to here as the *L_1/L_2 issue* and will be considered to be the prototype of a quasi-static optimization problem in that it fails to have a solution because the limiting process leads to a situation in which $\dot{x}$ has to be zero whereas its integral has to be one. Expressed somewhat differently, if the equations of motion are

$$\dot{x}_1 = u; \qquad \dot{x}_2 = u^2,$$

then the set of points reachable in infinite time is not a closed set. Points of the form $(x_1, x_2) = (a, 0)$ with $a \neq 0$ are in the closure of the set of points reachable from $(0, 0)$ in some finite time but are not reachable.

2.2. Infinitesimal bracketing

The issue here is more subtle. As an example, consider the equations of motion

$$\dot{x} = u; \qquad \dot{y} = v; \qquad \dot{z} = (xv - yu)/2;$$

with initial conditions $x(0) = x_0, y(0) = y_0, z(0) = 0$. Suppose we are given real numbers a and b such that $0 < b < y_0 < a$ and that $y(t)$ is subject to a state space constraint

$$b + kz(t) \leq y(t) \leq a - kz(t)$$

with $k > 0$. The problem is to choose u and v so as to maximize $z(1)$. Observe that if at some point $b + kz(t) = a - kz(t)$, i.e., if $z(1) = (a - b)/2k$, then z cannot be increased further because from that point on y is constant and the term $x\dot{y} - y\dot{x}$ integrates to zero around any closed path. We want to show that there exist trajectories that steer $z(t)$ from zero to any value of $z(1)$ which is slightly less than $(a-b)/2k$. Fig. 1 illustrates a somewhat more general situation in which the bounds on y are non necessarily affine. On the left it shows y as a function of z. The idea is that it is possible to increase $z(t)$ by letting x and y trace out a spiral-like motion consisting of a nested family of thin, vertically aligned, trapezoids.

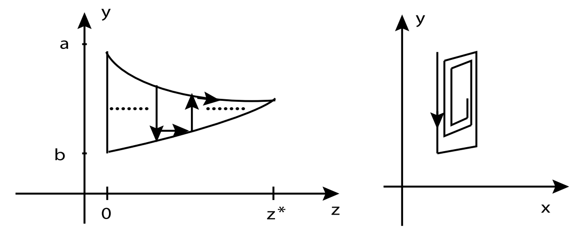

Fig. 1. Left: Illustrating a portion of a path in z–y-coordinates which generates an approximation to the limiting value of z. Right: Showing an approximating path in x–y coordinates.

Take the first of these to be of height $a - b$ and width δ, incorporating the slight deviation from a rectangle necessary to meet the constraint on y. Such a trapezoid generates an area which is, to first order in δ, $(a-b)\delta$. Having completed this path, the possible range for y is reduced to $b+k(a-b)\delta \leq y \leq a-k(a-b)\delta$, all to first order in δ. The subsequent trapezoids follow this pattern. In the limit as δ goes to zero the sum of the areas swept out equals the area of the triangle shown in Fig. 1 but because of the effect of the constraint on y, no nonzero width family completely fills the triangle. For example, if the sum of the accumulated areas were to completely fill the triangle both x and y would need to have infinite total variation. One can consider this to be a problem defined on any interval, finite or infinite, and the result is the same.

Lemma. *Let g_1 and g_2 be real valued functions, monotone decreasing and monotone increasing, respectively. Suppose that $g_1(0) > g_2(0)$ and suppose that there exists z^* such that $g_1(z^*) = g_2(z^*)$. Consider the system*

$$\dot{x} = u; \qquad \dot{y} = v; \qquad \dot{z} = (xv - yu)/2;$$

with initial conditions $x(0) = x_0, y(0) = y_0, z(0) = 0$. Assume that $y(t)$ is constrained in accordance with

$$g_2(z(t)) \leq y(t) \leq g_1(z(t));$$

Then the point $x = x(0), y = g_1(z^*), z = z^*$ is in the closure of the reachable set.

Proof. Consider cycles of the form shown in the right panel of Fig. 2 with the path constrained to be such that the y-coordinate lies between the limits defined by g_1 and g_2 and the x-coordinate is such that $|x(t) - x_0| \leq \Delta$. Each cycle adds approximately $(g_2(z) - g_1(z))\Delta$ to z until z is such that $g_2(z) = g_1(z)$. In the limit as Δ goes to zero this approximation becomes arbitrarily close to the given bound. ■

More generally, the possibility that the reachable set is not closed must be considered when investigating any system of the form $\dot{x} = \sum g_i(x)u_i$, with or without state space constraints.

3. A stochastic model for basic thermodynamics

Consider the model used in [6,7] to investigate Carnot efficiency. Fig. 2 illustrates a circuit containing a variable capacitor, two resistors and a three position switch. The resistors are assumed to be at temperatures T_1 and T_2, respectively, and to have an associated thermal noise consistent with the Nyquist–Johnson model [8]. In view of the central role played by energy, it is natural to write the stochastic differential equations describing the situation in terms of $\hat{x} = \sqrt{c}v$ where c is the (time dependent) value of the capacitance and v is the voltage across the capacitance. Without the noise term, the description of such a resistor–capacitor circuit is

$$\frac{d}{dt}cv = -gv; \quad g = \text{conductance}$$