Finite dimensional thermo-mechanical systems and second order constraints

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Abstract

In this paper we study a class of physical systems that combine a finite number of mechanical and thermodynamic observables. We call them finite dimensional thermo-mechanical systems. We introduce these systems by means of simple examples. The evolution equations of the involved observables are obtained in each example by using, essentially, the Newton’s law and the First Law of Thermodynamics only. We show that such equations are similar to those defining certain mechanical systems with higher order constraints. Moreover, we show that all of the given examples can be described in a variational formalism in terms of second order constrained systems.

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1 Introduction

Physical systems are essentially defined by observables and laws. Typically, the former are magnitudes whose values can be reached by experiments, and the latter are equations that determine and/or relate such values. If the time is involved in the description of the system (which can be seen as another observable), the relations between each observable and the time give precisely the evolution equations of the system. Roughly speaking, when the observables are positions and velocities, we say that we have a mechanical system. On the other hand, when such observables are the temperature, the pressure, the entropy, the volume and, for instance, the number of moles of certain chemical compounds, we say that we have a thermodynamic system. In this paper we shall study physical systems defined, at the same time, by observables of the two mentioned types: mechanical and thermodynamic observables. In other words, we shall study physical systems that combine mechanical and thermodynamic “degrees of freedom”. We shall call them thermo-mechanical systems. Only those with a finite number of observables will be considered here.

The paper is divided into two parts. The organization and the content are as follows. In the first part, in Section 2, we introduce the idea of thermo-mechanical system by means of several simple examples, i.e. we give some kind of ostensive definition of such systems. We focus our attention on finding, for each one of the given examples, the evolution equations of its corresponding observables. To do that, for the mechanical observables we only consider the Newton’s laws and for the thermodynamic observables we consider the First Law of Thermodynamics. Regarding the combination of such observables, we shall assume that the work made on the underlying thermodynamic system is due to the...
external (typically non-conservative) force acting on the mechanical counterpart. This gives rise to an Energy Conservation Principle which extends those of classical mechanics and thermodynamics. Such a principle adds another equation to the set of evolution equations. Among the solutions of the latter, we choose those for which the evolution of the thermodynamic observables satisfy the Second Law of Thermodynamics.

Since this kind of systems have not been extensively studied in the literature, we dedicate some effort on investigating their evolution equations. By doing that, we conclude that the systems under consideration can be described as mechanical systems with (higher order) constraints. This drives us to the second part of the paper, the Section 3 where a precise definition of a thermo-mechanical system is given inside a variational framework. More precisely, we define such systems as a particular subclass of the second order constrained systems (SOCS) [see [8, 13]]. We describe in this new formalism all the examples presented in the first part of the paper.

We assume that the reader is familiar with the fundamental concepts of thermodynamics (see [16, 19, 11, 6, 23]). However, a brief review of these concepts can be found in the Appendix. We also assume some familiarity with basic aspects of classical mechanics (see for instance [4, 12]). For the second part, a background on Differential Geometry (see [5, 14, 2]) and the ideas of Lagrangian and Hamiltonian systems in the context of the Geometric Mechanics (see [1, 15]) is expected.

2 (Examples of) Thermo-mechanical systems

By a thermo-mechanical system we shall mean a physical system that combines both mechanical and thermodynamic degrees of freedom, i.e. a physical system whose states are defined by mechanical observables, such as positions and velocities, and thermodynamic observables, e.g. temperature, entropy, pressure, volume, etc., such that the mentioned observables obey the laws of classical mechanics and thermodynamics. In the following, in order to grasp an idea of what kind of systems we are talking about, we introduce some examples (most of them originally presented in [3]). One of our aims is to find, for each one of these examples, the equations that determines the evolution of its corresponding observables.

2.1 Wagon with internal friction

Consider a wagon (chassis, axles and wheels) with mass $m$, whose wheels rolls with no sliding on a horizontal line. The wheels of the wagon are connected by pairs with an axle, rigidly attached to the wheels, that breaks through the wagon from side to side (see Figure 1). A friction force is present between each axle and the chassis and it is supposed to be proportional to their relative angular velocity. We shall consider two different situations.

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1By external force we mean any non-conservative force, or a conservative force whose corresponding potential energy is not included in what we consider the mechanical energy of the system.

2Physical systems whose states depend on mechanical and thermodynamic variables are more common in the domain of continuous media or fluid dynamics, but not in contexts where only a finite number of degrees of freedom are involved.
2.1.1 Thermally isolated wagon

Assume first that there is no heat exchange between the whole wagon and the environment. In other words, only adiabatic processes are allowed. The thermodynamic observables we consider for the system are the internal energy $U$, the entropy $S$ and the temperature $T$.

Recall that a review on basic concepts of thermodynamics can be found in the Appendix. We also assume that the only available thermodynamic processes are the quasi-static ones, in the sense that the state equations hold at every moment (see Remark [IV]). We also assume that $U = \nu T$, where $\nu > 0$ is the heat capacity of the wagon (which is assumed to be constant). Then, according to the First Law of Thermodynamics in its infinitesimal form [see Eq. (62)], which in this case reads $dU = T\,dS$, the mentioned observables must satisfy the following (state) equations at each instant of time

$$U = \nu T \quad \text{and} \quad S = \nu \ln \left( \frac{T}{T_0} \right) + S_0,$$

where $T_0$ and $S_0$ are constant.

Remark 1. As we emphasize in the Appendix, every thermodynamic system defines a contact manifold, and its corresponding state equations give rise to a Legendre submanifold of it. In this example, such a manifold is an open subset of $\mathbb{R}^3$ with the contact form $\theta := dU - T\,dS$ [see Eq. (57)], where $(-T, S, U)$ are the global Darboux coordinates, and the Legendre submanifold is defined by Eq. (1). This aspect of thermodynamic systems will be important in the second part of the paper.

For the mechanical counterpart, we assume that the wheels and the axles have negligible mass, so the only relevant mechanical observables are the position $x$ of the chassis and its time derivative $\dot{x}$. The Newton’s laws say that

$$m\ddot{x} = -\mu \dot{x},$$

being $\mu > 0$ a constant depending on the friction torque between the axle and the chassis (and also on the diameter of the wheels). Its general solution is

$$x(t) = -\frac{\dot{x}_0 m}{\mu} \left( e^{-\frac{\mu t}{m}} - 1 \right) + x_0.$$
This says that the internal friction of the axles will slow down the wagon exponentially, as expected.

Consider again the First Law of Thermodynamics [see Eq. (60)]. It says that the variation $\Delta U$ of the internal energy along any process is equal to the heat $Q$ exchanged between the wagon and the environment (along such a process) minus the mechanical work $W$ made on the wagon, i.e. $\Delta U = Q - W$. On one hand, by the adiabaticity condition assumed above, we know that $Q = 0$. On the other hand, the unique forces that make work are the friction forces between the axles and the chassis (the force exerted on the wheels by the floor, which allows the wheels to roll with no sliding, does not make work), and such a work is equal to $\Delta E_{\text{mec}}$, i.e. the variation of the mechanical energy $E_{\text{mec}} = m\dot{x}^2/2$.

**Remark 2.** As usual, a friction force acting on a mechanical system (see the right hand side of Eq. (2)) is conceived as an external force. Also, this kind of forces are non-conservative. This is why the mechanical energy $E_{\text{mec}}$ is given by the kinetic energy only.

Thus, $W = \Delta E_{\text{mec}}$, or equivalently $\Delta E_{\text{mec}} + \Delta U = 0$. Consequently, if we define the total energy of the system as

$$ E := E_{\text{mec}} + U = \frac{m\dot{x}^2}{2} + \nu T, \quad (4) $$

then $E$ is conserved for all $t$, namely [see (2)], the identity

$$ \frac{d}{dt} \left( \frac{m\dot{x}^2}{2} + \nu T \right) = m\ddot{x}\dot{x} + \nu \dot{T} = -\mu \dot{x}^2 + \nu \dot{T} = 0 \quad (5) $$

must hold. As a consequence $\dot{T} = \frac{\mu \dot{x}^2}{\nu}$, and from (3) we have that

$$ T(t) = -\frac{m\dot{x}_0^2}{2\nu} e^{-\frac{2\mu t}{m}} + T_0. \quad (6) $$

Therefore, using (1) and the last equation we have, for each initial condition, only one thermodynamic process $t \mapsto (T(t), S(t), U(t))$. Note that, since

$$ \dot{S} = \frac{\nu \dot{T}}{T} = \frac{\mu \dot{x}^2}{T}, $$

the entropy increases in time when the wagon moves, i.e. the Second Law of Thermodynamic holds for all of these processes. Moreover, such processes are (generically) irreversible. In fact, in an isolated system as it stands, a thermodynamic process is reversible if only if the change of entropy vanishes. In our example, this is only possible if the velocity of the wagon is zero.

Summing up, we have a thermo-mechanical system defined by the observables $x$, $\dot{x}$, $T$, $S$ and $U$, whose evolution equations are given by Equations (1), involving the thermodynamic observables, Eq. (2), involving the mechanical ones, and Eq. (5), linking both of them. All of these equations enable us, given an initial condition, to find a unique temporal evolution $t \mapsto (x(t), \dot{x}(t), T(t), S(t), U(t))$. 
2.1.2 The wagon in a thermal bath

Assume now that heat exchange by conduction, between the wagon and the environment, is permitted, and that the wagon is immersed in a thermal bath of (constant) temperature \( T_b \). The observables of the system \( x, \dot{x}, T, S \) and \( U \) will be again subjected to the Eqs. (1) and (2). But now the total energy [see Eq. (4)] is not conserved. In fact, as we discussed above, since \( \Delta U = Q - W \) and \( \Delta E_{\text{mec}} = W \), with \( W \) given by the friction forces, we have that \( \Delta E = \Delta E_{\text{mec}} + \Delta U = Q \), or in infinitesimal terms \( dE = dQ \) (see Eq. (61) in the Appendix).

If no further information is available for \( \bar{d}Q \), we can only say that the temporal evolution of the system is given by curves \( t \mapsto (x(t), \dot{x}(t), T(t), S(t), U(t)) \) satisfying (1), (2) and the Second Law of Thermodynamics [see Eq. (70)], which in this case says that \( dS \geq dE/T \).

Assume that the Fourier’s law holds, i.e. the heat exchanged by conduction along a time \( dt \), between a body at temperature \( T \) and a thermal bath at temperature \( T_b \), is given by \( dQ = \kappa A (T_b - T) \, dt \). Here \( \kappa > 0 \) is the conduction coefficient (assumed constant) and \( A \) is related to the area though which the heat flux takes place. For simplicity, we shall take \( A \) equal to 1. Then \( \dot{E} = -\kappa (T - T_b) \), i.e. [compare to Eq. (5)]

\[
-\mu \ddot{x}^2 + \nu \dot{T} = -\kappa (T - T_b). \tag{7}
\]

As a consequence, under such assumptions, the evolution equations are (1), (2) and (7), and they determinate completely the evolution of all the observables. The solutions to (2) and (7) are given by (3) and

\[
T(t) = \left( T_b - T_0 - \frac{m \dot{x}_0^2}{2\nu} \right) e^{-\frac{\kappa}{\nu} t} - \frac{m \dot{x}_0^2}{2\nu} e^{-\frac{\kappa}{\nu} t} + T_b, \tag{8}
\]

respectively. Then \( S(t) \) and \( U(t) \) can be constructed by combining (1) with (8). Note that, according to (7),

\[
dS = \frac{\nu \dot{T}}{T} \, dt = \frac{\mu \ddot{x}^2}{T} \, dt + \kappa \left( \frac{T_b}{T} - 1 \right) \, dt \geq \kappa \left( \frac{T_b}{T} - 1 \right) \, dt = \frac{dQ}{T},
\]

what implies that each curve \( t \mapsto (T(t), S(t), U(t)) \) satisfies the Second Law and defines an irreversible process (at least when the wagon moves). In particular, above assumptions, including the Fourier’s law, are compatible with the Second Law of Thermodynamics.

**Remark.** Eqs. (1), (2) and (5) [resp. (7)] define a system of differential-algebraic equations, as those appearing in mechanical systems with constraints. This observation will be further exploited in Section 3.

2.2 Vertical piston

Consider an ideal gas (made of one chemical compound) confined in a cylinder by a vertical piston of mass \( m \) (see Figure 2). We shall consider two different kind of allowed processes.
2.2.1 Adiabatic processes

Assume that the piston and the cylinder, i.e. the container of the gas, are perfect thermal insulators and that there is no friction between them. The only mechanical observables are the piston’s position \( x \) and velocity \( \dot{x} \). Since the number of moles \( N \) of the gas is constant, say \( N := N_0 \), the relevant thermodynamic extensive variables are the internal energy \( U \), the volume \( V \) and the entropy \( S \), and the intensive ones are the pressure \( P \) and the temperature \( T \) of the ideal gas. It can be shown that these observables are related by the equations [see (67)]

\[
P V = N_0 RT, \tag{9}
\]

\[
U = \alpha N_0 RT \tag{10}
\]

and

\[
S = S_0 + N_0 R \ln \left( \frac{T^\alpha V}{T_0^\alpha V_0} \right), \tag{11}
\]

where \( S_0, V_0 \) and \( T_0 \) are constant with units of entropy, volume and temperature, respectively. Since the container of the gas is a thermal insulator, only adiabatic processes are allowed. As a consequence, the identity

\[
PV^\gamma = k \tag{12}
\]

also holds, where \( k \) is a constant and \( \gamma = \frac{\alpha + 1}{\alpha} \). Then, Equations (9), (11) and (12) imply that all processes must be isoentropic (as it is well known for the ideal gas), i.e.

\[
S = S_0, \tag{13}
\]

and consequently reversible. In summary, the thermodynamic observables must fulfill the Eqs. (9), (10), (12) and (13). Note that the Second Law is automatically satisfied.

Remark 3. For further convenience, and regarding the contact structure related to every thermodynamic system (see the Appendix), let us mention that the equations (9), (10) and (11) define a Legendre submanifold \( \mathcal{N} \subset \mathbb{R}^5 \), w.r.t. the contact form \( \theta := dU - T dS + P dV \) [see Eq. (57)], which encodes the equilibrium states of the ideal gas. The additional equation (13) gives a submanifold of \( \mathcal{N} \) where the adiabatic processes of the ideal gas are contained.
On the mechanical side, from Newton’s laws, the position $x$ of the piston must satisfy

$$m\ddot{x} = -mg + \frac{PA_{g}}{F_{e}},$$

(14)

where $A$ is the area of the horizontal section of the piston and $g$ is the acceleration of gravity, so the force associated is labeled $F_{g}$. Note that the force made by the pressure is an external force, from the point of view of the mechanical degrees of freedom, so we label it $F_{e}$. Because of the geometric configuration, we have that

$$Ax = V,$$

(15)

then, using Eq. (12), follows that

$$P = \frac{k}{(Ax)^{\gamma}},$$

(16)

As a consequence,

$$m\ddot{x} = F_{g} + F_{e} = -mg + \frac{kA}{(Ax)^{\gamma}}.$$

(17)

The solutions of the last equation are given by the quadrature

$$\int_{1}^{x(t)} \frac{\sigma}{\sqrt{c_{1} + 2 \left(-gs + \frac{kA}{mA^{\gamma}(1 - \gamma)} s^{1-\gamma}\right)}} ds = t + c_{2}.$$

(18)

Here, $c_{1}$ and $c_{2}$ are integration constants, and $\sigma = \pm 1$ (depending on the initial conditions). On the other hand, plugging the identity $Ax = V$ on Equations (9) and (10), we have that

$$T = \frac{k (Ax)^{1-\gamma}}{N_{0}R} \quad \text{and} \quad U = \alpha k (Ax)^{1-\gamma}.$$

(19)

Thus, as in the previous example, for each initial value of the mechanical observables we have only one (adiabatic) thermodynamic process, defined by a time-parametrized curve

$$t \mapsto (P(t), T(t), V(t), S(t), U(t)),$$

(20)

with [see Eqs. (13), (16) and (19)]

$$\begin{align*}
P(t) &= k (Ax(t))^{-\gamma}, \\
T(t) &= \frac{k (Ax(t))^{1-\gamma}}{N_{0}R}, \\
V(t) &= Ax(t), \\
S(t) &= S_{0}, \\
U(t) &= \alpha k (Ax(t))^{1-\gamma},
\end{align*}$$

(21)

and where $x(t)$ is given by the Eq. (18). As we said above, since the process is adiabatic and isoentropic, then it is reversible.
In conclusion, this example consists in a thermo-mechanical system defined by observables $x, \dot{x}, P, T, V, S$ and $U$, with evolution equations given by (17), mainly related to the mechanical degrees of freedom, the Eqs. (9), (10), (12) and (13), exclusively related to the thermodynamic ones, and the Eq. (15) that links both of them. In the next subsection we shall analyze a little bit closer the solutions of these equations.

2.2.2 Reversibility and quasi-staticity

It is easy to show that Eq. (17) is equivalent to the system of first order ordinary differential equations

$$\begin{align*}
\dot{q} &= \frac{p}{m}, \\
\dot{p} &= -mg + kA^{-\gamma+1}q^{-\gamma}.
\end{align*}$$

Such a system defines a Hamiltonian vector field with Hamiltonian function

$$H(q, p) := \frac{p^2}{2m} + mgq + \frac{\alpha k}{A^{\gamma-1}}q^{-1-\gamma}. \quad (22)$$

As it is well known, the Hamiltonian is conserved along the solutions. This conservation property will be analyzed in Section 2.2.4. Regarding its stability, it can be shown that the only equilibrium point is

$$(q^*, p^*) = \left(\frac{kA^{1-\gamma}}{mg}, 0\right),$$

which is a center. In the neighborhood of such center the solutions are closed orbits. For instance, when $m = 1, g = 1, A = 1, \alpha = \frac{3}{2}, \gamma = \frac{5}{3}$ and $k = 1$, we have the behavior shown in Figures 3 and 4. As a consequence, the solutions $x$ of Eq. (17) are oscillatory. This implies that all the observables of the system have an oscillatory behavior [recall Eq. (21)], which is consistence with the fact that, as we said before, each thermodynamic process (one for each initial condition) defined by (20) is reversible. Also, as it is known, near the equilibrium, speeds are slow. Then, around such a point, the quasi-static condition is satisfied in the usual sense (see Remark IV).
2.2.3 Isothermal processes

Assume now that, instead of the adiabaticity condition (12), we ask the temperature of the gas to be constant. Thus, the observables of the system \( x, \dot{x}, P, T, V, S \) and \( U \) satisfy again the Equations (9), (10), (11), (17) and (15), but (12) [or equivalently (13)] must be replaced by the condition \( T = T_0 \). In this case, Eq. (17) translates to

\[
m\ddot{x} = -mg + \frac{N_0RT_0}{x}.
\]

Solving this equation, we have for the rest of the observables the following expressions:

\[
\begin{align*}
P(t) &= \frac{N_0RT_0}{Ax(t)}, \\
T(t) &= T_0, \\
V(t) &= Ax(t), \\
S(t) &= S_0 + N_0R \ln \left( \frac{x(t)}{x_0} \right), \\
U(t) &= \alpha N_0RT_0,
\end{align*}
\]

being \( x_0 \) the initial position of the piston.

Remark 4. As in the adiabatic case, since the solutions of Eqs. (23) are invariant by changing \( t \) by \( -t \), then the curves given by Eqs. (24) define reversible processes.

2.2.4 The total energy conservation

Let us go back to Section 2.2.1 (the adiabatic case of the vertical piston). It can be shown by direct calculations that the quantity \( E := E_{mec} + U := \frac{m\dot{x}^2}{2} + mgx + U \) [compare to Eq. (22)]

\[
\text{[compare to Eq. (4)], that we can call the total energy of the system, is conserved along the curves that solve the Eqs. (9), (10), (12), (13), (17) and (15).}
\]

Remark. Note that we are considering that \( E_{mec} \) is constituted by, besides the kinetic energy, just the potential energy related to \( F_g = -mg \). We are not including the potential energy related to \( F_e = kA^{-\gamma+1}x^{-\gamma} \) because, as previously mentioned, we are taking it as an external force.

Moreover, it is easy to show that the last system of equations is equivalent (modulo an additive integration constant) to the systems given by Eqs. (9), (10), (12), (13), (17) and (15) and the condition \( \dot{E} = 0 \), i.e.

\[
m\ddot{x} \dot{x} + mg \dot{x} + \dot{U} = 0.
\]

That is to say, the equation given by the geometrical constraint between the position \( x \) and the volume \( V \) can be replaced by an energy conservation condition. Let us analyze why this conservation holds.

On one hand, the First Law of Thermodynamics says that \( \Delta U = Q - W \) [see Eq. (60)]. In the system under consideration, \( Q = 0 \) and \( W \) is the work made by the pressure of the
gas. In particular \( \Delta U = -W \). On the other hand, by the laws of classical mechanics, the variation \( \Delta E_{\text{mec}} \) of the mechanical energy is equal to the work made by the external forces acting on the underlying mechanical system, which in this case (see previous Remark) is given by the pressure of the gas. Then \( \Delta E_{\text{mec}} = W \), and consequently \( \Delta E_{\text{mec}} + \Delta U = 0 \). So the total energy conservation property is due to the fact that:

\[ W \text{ the work made on the underlying thermodynamic system is precisely the work made by the external forces acting on the underlying mechanical counterpart. } \]

In other words, the internal energy \( U \) is defined by the work of the external forces appearing in the underlying mechanical system (see Remark IV). Notice that the same is true for the wagon with internal friction (see Remark 2 and the paragraph before it).

Now, let us go back to Section 2.2.3. If we calculate the derivative of the total energy \( E \) [see Eq. (25)] along the curves solving Eqs. (23) and (24), we obtain that \( \dot{E} = T_0 \dot{S} \), i.e.

\[ m\ddot{x} + mg\dot{x} + U = T_0 \dot{S}. \]

(27)

In particular, the total energy is not conserved in this case. Let us mention that, contrary to what happens for the adiabatic situation, the geometrical condition in Eq. (15) can not be replaced by Eq. (27).

**Remark.** Since the statement \( W \) holds in this case too, we have that \( \Delta U = Q - W \) and \( \Delta E_{\text{mec}} = W \), and since \( \Delta U = 0 \) (because \( U = \alpha N_0 R T_0 = \text{cte} \)), then \( \Delta E = \Delta E_{\text{mec}} = Q \). So, from the identity \( \dot{E} = T_0 \dot{S} \), or equivalently \( \Delta E = T_0 \Delta S \), we have that \( \Delta S = Q/T_0 \). This implies that all the involved processes satisfy the Second Law and are reversible, as mentioned in Remark 4 [see also Eq. (71)].

We shall assume from now on that statement \( W \) holds for all the thermo-mechanical systems we consider in this paper. This is clearly equivalent to the following extension of the Energy Conservation Principle:

**ECP** Consider a thermo-mechanical system whose underlying mechanical (resp. thermodynamic) system has energy \( E_{\text{mec}} \) (resp. \( U \)). If, along a given process, the heat \( Q \) exchanged between the underlying thermodynamic system and the environment is zero, then the total energy \( E := E_{\text{mec}} + U \) is preserved, i.e. \( \Delta E_{\text{mec}} + \Delta U = 0 \). In general, we shall have that \( \Delta E_{\text{mec}} + \Delta U = Q \).

### 2.3 Dissipative vertical piston

Consider again the gas, the cylinder and the piston, but this time suppose that there exists friction between the cylinder and the piston. In addition, suppose that dissipation by conduction is present between the gas and its container (cylinder and piston). As in Section 2.2.1 we assume that no heat exchange takes place between the container and the environment. We model the mentioned friction in the same way as we did for the wagon, where the massless cylinder and the massive piston would play the role of the massless axles and the massive chassis, respectively. Shortly speaking, we are considering a sort of combination of the main features of the thermo-mechanical systems studied in Sections 2.1 and 2.2.

The observables in this case are:
a) the position \( x \) and velocity \( \dot{x} \) of the piston;

b) the internal energy \( U_c \), the temperature \( T_c \) and the entropy \( S_c \) of the whole container (i.e. the cylinder and the piston), for which we assume (as we did for the wagon) that \( U_c = \nu T_c \);

c) the internal energy \( U \), the pressure \( P \), the volume \( V \), the temperature \( T \) and the entropy \( S \) of the ideal gas.

Note that, with respect to the last example, new thermodynamic variables are present. Moreover, we can see this new example as a composite system (see Remark [1], with subsystems given by the “container” and the “gas”. In particular, the internal energy of the whole underlying thermodynamic system is \( U + U_c = U_{\text{tot}} \).

Allowing again only quasi-static processes, the thermodynamic observables must satisfy, at every time, the state equations

\[
U_c = \nu T_c \quad \text{and} \quad S_c = \nu \ln \left( \frac{T_c}{T_{c,0}} \right) + S_{c,0} \tag{28}
\]

for the container, and

\[
PV = N_0 RT, \quad U = \alpha N_0 RT \quad \text{and} \quad S = S_0 + N_0 R \ln \left( \frac{T^0 V}{T^0_0 V_0} \right) \tag{29}
\]

for the gas. On the mechanical side, we have that

\[
m\ddot{x} = -mg + PA - \mu \dot{x}, \tag{30}
\]

where \( \mu \) is the friction coefficient between the cylinder and the piston, which we are assuming constant. Recalling that

\[
V = Ax \tag{31}
\]

and using the first formula of Eq. (29), we have that

\[
PA = \frac{N_0 RT}{x},
\]

so Eq. (30) translates to

\[
\dot{m} \ddot{x} = -mg + \frac{N_0 RT}{x} - \mu \dot{x}. \tag{32}
\]

On the other hand, since there is no heat exchange between the whole system (container plus gas) and the environment, assumption ECP (see at the end of Section 2.2.4) says that the total energy

\[
E = E_{\text{mec}} + U + U_c = \frac{m \dot{x}^2}{2} + mgx + \alpha N_0 RT + \nu T_c
\]

must be conserved, i.e.

\[
(m \ddot{x} + mg) \dot{x} + \alpha N_0 R \dot{T} + \nu \dot{T}_c = 0. \tag{33}
\]
As for the wagon in a thermal bath, if no further information is given for heat transferred per time unit, we cannot determine completely the evolution. We can only say that it is given by curves satisfying the Equations (28), (29), (31), (32) and (33), and the Second Law.

Assume again that the Fourier’s law holds. Let us consider the subsystem formed out by the container (cylinder and piston). According to such law (as seen in Section 2.1.2), the variation \( \dot{E}_{\text{mec}} + \dot{U}_c \) of its total energy per time unit must be equal to \(-\kappa A (T - T_c)\) (the heat transferred per time unit), that is to say

\[
(m\ddot{x} + mg) \dot{x} + \nu \dot{T}_c = \kappa A (T - T_c),
\]

where \(\kappa\) is the conduction coefficient (which we assume constant) and \(A\) is the area through which heat flows, which is a linear function on \(x\). Combining the last equation with (33), it follows that

\[
\dot{T} = \frac{\kappa A}{\alpha N_0 R} (T_c - T).
\]

The system of ordinary differential equations given by Eq. (32), (33) and (35) determine completely the evolution of the observables \(x, T\) and \(T_c\). It is clear that the evolution of the rest of observables can be derived from Eqs. (28), (29) and (31).

To visualize the behavior of this system [see Figures 5 and 6], we solve numerically\(^iv\) the Equations (35), (32) and (33) (for the unknowns \(T, T_c\) and \(x\)) in the case in which \(g = 9, m = 1, \kappa = 0.2, \mu = 0.8, \nu = 0.5, N_0 R = 1, \alpha = 3/2\) and with initial conditions \(x(0) = 15, \dot{x}(0) = 0, T(0) = 25\) and \(T_c(0) = 20\). In Figure 5 the red curve is the temperature of the ideal gas, the blue one is the position of the piston, and the yellow one is the temperature of the container.

The evolution of the entropies is shown in Figure 6, where we are setting \(S_0 = 0 = S_{c,0}\). The red curve is the total entropy \(S(t) + S_c(t)\), the blue one is \(S(t)\) and the yellow is \(S_c(t)\). In such a figure, it can be seen the monotonic behavior of the total entropy, which agrees with the statement of the Second Law of Thermodynamics.

Remark. It might happen, for another choice of parameters, that some curves do not satisfy the Second Law. In such a case, we must select those curves that do fulfill such law.

To summarize, this thermo-mechanical system is defined by observables \(x, T_c, S_c, U_c, P, T, V, S\) and \(U\), subjected to the Eq. (30) for the mechanical side, the Eqs. (28), (29) and (35) for the thermodynamic counterpart, and Eqs. (31) and (33) coupling the previous ones.

Remark. It is well known that Fourier’s law of heat conduction is empirical, so unlike previous examples where the validity of the Second Law of Thermodynamics may be inferred by construction or simply calculations, in this example it is not obvious that the total entropy of the system increases in time; fact shown in Figure 6.

\(^iv\)Using NDSolve in Wolfram Mathematica.
3 Thermo-mechanical systems and constraints

We saw in the previous section that the observables of a thermo-mechanical system satisfy a set of differential-algebraic equations as those appearing in mechanical systems with constraints. In this section we are going to show that such equations can be seen as the equations of motion of a constrained Lagrangian system, on a finite-dimensional manifold, as those defined in [8]: the second order constrained systems (SOCS). We shall do that within a variational formalism.

Also, we shall show that the manifold on which each SOCS is defined is a product of two manifolds: one of them related to the underlying mechanical system, and the other to the thermodynamic counterpart. The latter, as stood out in Remarks 1 and 3, is a contact manifold.

3.1 Second order constrained systems (SOCS)

In [8], a class of Lagrangian systems with higher order constraints has been studied. Let us recall the definition of such systems in the second order case.

Fix a smooth $n$-manifold $Q$ and a function $L : TQ \to \mathbb{R}$. As usual, we shall say that $(Q, L)$ is a Lagrangian system and $L$ is its Lagrangian function. Given a curve $\gamma : [t_1, t_2] \to Q$, recall that an infinitesimal variation of $\gamma$ with fixed end points, or simply a variation of $\gamma$, is a curve $\delta \gamma : [t_1, t_2] \to TQ$ such that $\delta \gamma(t) \in T_{\gamma(t)}Q$, for all $t \in [t_1, t_2]$, and $\delta \gamma(t_1, 2)$ belongs to the null distribution of $Q$. In particular, $\gamma = \tau \circ \delta \gamma$, being $\tau : TQ \to Q$ the canonical tangent bundle projection. By $\gamma' : [t_1, t_2] \to TQ$ and $\gamma^{(2)} : [t_1, t_2] \to T^{(2)}Q$ we shall denote the velocity and the acceleration of $\gamma$, respectively,
and by $\delta \gamma' : [t_1, t_2] \to TTQ$ the velocity of $\delta \gamma$. Here $T^{(2)}Q$ denotes the second order tangent bundle of $Q$ (see [10]).

**Definition 3.1.** Let us consider the triples $(L, C_K, C_V)$ with

$$C_K \subset T^{(2)}Q \quad \text{and} \quad C_V \subset TQ \times_Q TQ,$$

where $C_K$ is a submanifold and $C_V$ is such that, for every $v \in TQ$, the intersection

$$C_V(v) \equiv C_V \cap \{v\} \times T\tau(v)Q,$$

naturally identified with a subset of $T\tau(v)Q$, is empty or a linear subspace. We shall refer to these triples as **second order constrained systems (SOCS)**, with Lagrangian function $L$, **kinematic constraints** $C_K$ and **variational constraints** $C_V$. We shall say that $\gamma : [t_1, t_2] \to Q$ is a **trajectory** of $(L, C_K, C_V)$ if the following conditions are satisfied

1. $\gamma^{(2)}(t) \in C_K, \forall t \in (t_1, t_2)$;
2. for all variations $\delta \gamma$ such that $(\gamma'(t), \delta \gamma(t)) \in C_V$,

$$\int_{t_1}^{t_2} \langle dL(\gamma'(t)), \kappa(\delta \gamma'(t)) \rangle \ dt = 0,$$

where $\kappa : TTQ \to TTQ$ is the canonical involution (see [22]).

Let us describe such triples and their related equations in local terms. Consider a local chart $(U, \varphi)$ of $Q$, with $\varphi : U \to \mathbb{R}^n$. Given $q \in U$ and $v \in T_qU$, write $\varphi(q) = (q^1, \ldots, q^n)$ and

$$\varphi_*(v) = (q^1, \ldots, q^n, \dot{q}^1, \ldots, \dot{q}^n) \quad \text{or} \quad \varphi_*(v) = (q^1, \ldots, q^n, \delta q^1, \ldots, \delta q^n),$$

(37)
where $\varphi_* : T\mathcal{U} \to \mathbb{R}^n \times \mathbb{R}^n$ is the differential of $\varphi$ (under usual identifications). Sometimes, we shall also use $q$ and $(q, \dot{q})$ or $(q, \delta q)$ in order to denote $\varphi(q)$ and $\varphi_*(v)$, respectively, just for brevity. In this notation, for the local representative of $\tau$ we have that
\[
\tau(q, \dot{q}) = \tau(q, \delta q) = q.
\]
For a curve $\gamma : [t_1, t_2] \to Q$, write
\[
\varphi(\gamma(t)) = (q^1(t), ..., q^n(t)) = q(t),
\]
\[
\varphi_*(\gamma'(t)) = (q^1(t), ..., q^n(t), \dot{q}^1(t), ..., \dot{q}^n(t)) = (q(t), \dot{q}(t)),
\]
\[
\varphi_*(\delta \gamma(t)) = (q^1(t), ..., q^n(t), \delta q^1(t), ..., \delta q^n(t)) = (q(t), \delta q(t)),
\]
in the open set where $\varphi \circ \gamma$ is defined. Finally, for a point $\eta \in T_q^{(2)}Q$, write
\[
\varphi^{(2)}(\eta) = (q^1, ..., q^n, \dot{q}^1, ..., \dot{q}^n, \ddot{q}^1, ..., \ddot{q}^n) = (q, \dot{q}, \ddot{q}),
\]
and for a curve $\gamma$,
\[
\varphi^{(2)}(\gamma^{(2)}(t)) = (q^1(t), ..., q^n(t), \dot{q}^1(t), ..., \dot{q}^n(t), \ddot{q}^1(t), ..., \ddot{q}^n(t)) = (q(t), \dot{q}(t), \ddot{q}(t)),
\]
where $\varphi^{(2)} : T^{(2)}\mathcal{U} \to \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n$ is the 2-lift of $\varphi$ (again, under usual identifications). In these terms, given a triple $(L, C_K, C_V)$, if $C_K$ is a regular submanifold and $C_V$ is such that the subspaces $C_V(v)$ depends smoothly on $v$, then such subsets are locally given by equations of the form
\[
w^a(q, \dot{q}, \ddot{q}) = 0 \quad \text{and} \quad v^b_i(q, \dot{q}) \delta q^i = 0,
\]
respectively, for certain functions $w^a$'s and $v^b_i$'s (sum over repeated indices convention is assumed form now on). As a consequence, a curve $\gamma$ is a trajectory of the triple if and only if
1. $w^a(q(t), \dot{q}(t), \ddot{q}(t)) = 0$,
2. and, as it is easy to show,
\[
\left( \frac{d}{dt} \left( \frac{\partial (L \circ \varphi^{-1}_*)}{\partial \dot{q}^i} (q(t), \dot{q}(t)) \right) \right) \delta q^i(t) = 0 \quad (38)
\]
for all functions $\delta q^i$ such that
\[
v^b_i(q(t), \dot{q}(t)) \delta q^i(t) = 0.
\]
Eq. (38) is called generalized Lagrange-D’Alembert equation.

**Definition 3.2.** Given $v \in TQ$ such that $C_V(v)$ is not empty, define
\[
F_V(v) = (C_V(v))^\perp \subset T^*_{v}Q.
\]
The union of the subsets $\{v\} \times F_V(v)$ defines a subset $F_V \subset TQ \times Q^*TQ$, that we will call the space of **constraint forces**.
Remark. Since $C_V$ and $F_V$ are related by annihilation, both of them contain the same information. So, we can also describe the SOCSs as triples $(L, C_K, F_V)$.

Particular examples of SOCSs are the holonomic and the nonholonomic systems (see [8, 13]). Indeed, consider a nonholonomic system defined by a Lagrangian function $L$ and a set of constraints given by a distribution $D \subset TQ$. Define $C_K := (\tau^{(1,2)})^{-1}(D)$ and $C_V := TQ \times Q \, D$, where $\tau^{(1,2)} : T^{(2)}Q \rightarrow TQ$ is the canonical projection (in coordinates, $\tau^{(1,2)}(q, \dot{q}, \ddot{q}) = (q, \dot{q})$). Then $(L, C_K, C_V)$ is a SOCS whose trajectories, with initial conditions inside $D$, coincide with those of the given nonholonomic system. In the case of a holonomic system with constraints given by a submanifold $Q_1 \subset Q$, define $C_K := \tau^{(1,2)}(D)$ and $C_V := TQ_1 \times Q_1 \, TQ_1$. Again, the related SOCS has the same trajectories as the mentioned holonomic system (for initial conditions inside $TQ_1$), i.e. the same trajectories as the Lagrangian system $(Q_1, L|_{TQ_1})$. Following similar ideas, generalized nonholonomic systems (GNHS) (see [7] and [8]) can also be seen as SOCSs.

Remark. Notice that for nonholonomic systems, given $q \in Q$ and $v \in T_qQ$, we have that $C_V(v) = D_q$. Consequently, $F_V(v) = D_q$, that is, the constraint forces vanish on the allowed velocities, which is the content of the D’Alembert’s Principle.

In what follows, we shall see that the thermo-mechanical systems presented in Section 2 can be seen as SOCSs.

3.2 Wagon with internal friction revisited

Let $Q = \mathbb{R} \times \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}$, where $\mathbb{R}^+$ is the set of positive real numbers, denote by $(x, T, S, U)$ the points of $Q$ and define $L : TQ \rightarrow \mathbb{R}$ as

$$L(x, T, S, U, \dot{x}, \dot{T}, \dot{S}, \dot{U}) = \frac{m \dot{x}^2}{2} - U,$$

with $m$ a positive constant. For the Lagrangian system $(Q, L)$, consider the second order kinematic constraints $C_K \subset T^{(2)}Q$ given by the points

$$\left(x, T, S, U, \dot{x}, \dot{T}, \dot{S}, \dot{U}, \ddot{x}, \ddot{T}, \ddot{S}, \ddot{U}\right)$$

such that

$$U = \nu T, \quad S = S_0 + \nu \ln \left(\frac{T}{T_0}\right) \quad \text{and} \quad m \ddot{x} \dot{x} + \dot{U} = 0,$$

where $\nu$, $T_0$ and $S_0$ are positive constant. If $m$ and $\nu$ are the mass and the specific heat of the wagon presented in Section 2.1.1, it is clear that $L$ is the difference between its kinetic and its internal energy, and the equations in (41) correspond to the state equations of the thermodynamic counterpart and the conservation of the total energy $E$ of the wagon [see Eq. (5)].
Finally, consider the variational constraints \( C_V \subset TQ \times QTQ \) defined by the points
\[
(x,T,S,U,\dot{x},\dot{T},\dot{S},\delta x,\delta T,\delta S,\delta U)
\]
such that
\[
\delta U = \nu \delta T, \quad \delta S = \nu \frac{\delta T}{T} \quad \text{and} \quad \mu \dot{x} \delta x = \delta U,
\]
with \( \mu \) another positive constant. If \( \mu \) is the friction coefficient between the axles and the chassis of the wagon, the last equation say that the infinitesimal variation of the internal energy \( U \) of the wagon is due to the infinitesimal work made by the friction force.

It can be shown that the trajectories of the triple \((L,C_K,C_V)\) are in bijection with the curves \( t \mapsto (x(t),\dot{x}(t),T(t),S(t),U(t)) \) found in Section 2.1.1. In fact, the generalized Lagrange-D’Alembert Equation \( (38) \) for \((L,C_K,C_V)\) reduces to
\[
-\text{m} \ddot{x} \delta x - \delta U = 0.
\]
Using the latter and the variational constraint \( \mu \dot{x} \delta x = \delta U \) [see Eq. \((42)\)], the Newton’s equation for the wagon \( m \ddot{x} = -\mu \dot{x} \) follows [recall Eq. \((2)\)]; and using the kinematic constraints given by Eq. \((41)\), we have the Eqs. \((1)\) and \((5)\). In conclusion, we can describe the thermo-mechanical system presented in Section 2.1.1 as the SOCS \((L,C_K,C_V)\) given by Eqs. \((40), (41)\) and \((42)\). A similar assertion can be made about the thermo-mechanical system of Section 2.1.2, provided we assume the Fourier law holds. We just must replace the condition \( m \ddot{x} \dot{x} + \dot{U} = 0 \) by [recall Eq. \((7)\)]
\[
m \ddot{x} \dot{x} + \dot{U} = \kappa (T_b - T).
\]
In both cases, the Second Law is automatically satisfied.

On the other hand, if no further information is given for the heat exchange, then we do have a SOCS again, but its equations of motion do not determine completely the trajectories. In addition, in such a case, we must ask the trajectories to satisfy the Second Law.

To end this subsection, note that the manifold \( Q \) can be written as a Cartesian product of two manifolds: \( M = \mathbb{R} \), related to the mechanical degrees of freedom, and \( T = \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R} \times \mathbb{R} \), related to the thermodynamical ones (namely \( U, T \) and \( S \)). The latter, as explained in Remark \( 1 \) is a 3-dimensional contact manifold with contact form \( \theta = dU - T dS \). Note also that some of the conditions that define \( C_K \), the state equations, give rise to a Legendre submanifold of \( T \). As we shall see below, this is not a peculiarity of the present example, but a common characteristic of all the examples we introduced in this paper.

3.3 Vertical piston revisited

3.3.1 The adiabatic case

Let \( Q = \mathbb{R} \times \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R} \), denote by \((x,P,T,V,S,U)\) the points of \( Q \) and define \( L : TQ \to \mathbb{R} \) as
\[
L \left( x,P,T,V,S,\dot{x},\dot{P},\dot{T},\dot{V},\dot{S},\dot{U} \right) = \frac{m\dot{x}^2}{2} - mgx - U,
\]
with $m$ and $g$ positive constants. Consider the submanifold $C_K \subset T^{(2)}Q$ given by the equations

$$PV = N_0RT, \quad U = \alpha N_0RT, \quad Ax = V, \quad (44)$$

$$S = S_0 \quad \text{and} \quad PV^\gamma = k, \quad (45)$$

and $C_V \subset TQ \times_Q TQ$ given by

$$\delta PV + P \delta V = N_0R \delta T, \quad \delta U = \alpha N_0R \delta T, \quad A \delta x = \delta V, \quad (46)$$

$$\delta S = 0 \quad \text{and} \quad \delta PV^\gamma + \gamma PV^{\gamma-1} \delta V = 0,$$

where $N_0$, $R$, $\alpha$, $S_0$, $k$ and $A$ are positive constants, and $\gamma = \frac{\alpha+1}{\alpha}$.

The generalized Lagrange-D’Alembert equation for $(L, C_K, C_V)$ is

$$-m \ddot{x} \delta x - mg \delta x - \delta U = 0.$$

Using the variational constraints, it is easy to show that $\delta U = -P \delta V = -PA \delta x$. Then, the equation above reduces to

$$-m \ddot{x} - mg + PA = 0.$$

This equation together with the kinematic constraints in Eqs. (44) and (45) are exactly the Equations (9), (10), (12), (13), (17) and (15) obtained for the thermo-mechanical system presented in Section 2.2.1. Thus, the adiabatic vertical piston is a SOCS.

Remark. Note that Eqs. (44) and (45) defines a submanifold $Q_1 \subset Q$ in terms of which we can define

$$C_K := (\tau^{(1,2)})^{-1}(TQ_1) \quad \text{and} \quad C_V (v) := T_q Q_1,$$

for all $q \in Q_1$ and $v \in T_q Q$. Taking into account the discussion around Eq. (39), the equation above says that the SOCS $(L, C_K, C_V)$ can be seen as a holonomic system (with constraints given by $Q_1$), i.e. it is equivalent to the Lagrangian system $(Q_1, L|_{TQ_1})$. Since, in addition, $L|_{TQ_1}$ is hyperregular, such a HOCS is equivalent to a Hamiltonian system, as it was established in Section 2.2.2.

Recall that condition $Ax = V$ can be replaced by the conservation of the quantity

$$E = \frac{m \dot{x}^2}{2} + mgx + U,$$

[see Section 2.2.4], which gives the second order constraint

$$m \ddot{x} + mg \dot{x} + \dot{U} = 0$$

[see Eq. (26)]. It can be shown that, if we change $Ax = V$ by the equation above, and change $A \delta x = \delta V$ by

$$-PA \delta x = \delta U,$$

the new SOCS has the same trajectories as the previous one. The last equation says that the infinitesimal variation of the internal energy is due to the infinitesimal work made by the pressure.

As in the previous example, let us note that the manifold $Q$ can be written as a Cartesian product of two manifolds. In this case, $\mathcal{M} = \mathbb{R}$ and $\mathcal{T} = \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}$, where the latter is a contact manifold with global Darboux coordinates $(P, -T, V, S, U)$ and contact form $\theta = dU - T dS + P dV$.

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3.3.2 The isothermal case

Take $Q$ and $L$ as above, and define $C_K \subset T^{(2)}Q$ by the equations \(44\) plus
\[
S = S_0 + N_0 R \ln \left( \frac{T V}{T_0 V_0} \right), \quad T = T_0 \tag{47}
\]
and [see Eq. \(27\)]
\[
m\ddot{x} + mg \dot{x} + \dot{U} = T \dot{S}.
\]
Finally, define $C_V \subset TQ \times Q$ by the equations \(46\) plus
\[
\delta S = N_0 R \left( \frac{\delta V}{V} - \alpha \frac{\delta T}{T} \right), \quad \delta T = 0 \tag{48}
\]
and
\[-PA \delta x = \delta U.\]

Again, $N_0$, $R$, $\alpha$, $T_0$, $S_0$, $V_0$ and $A$ are positive constants. Note that all the variations must vanish. So, the generalized Lagrange-D’Alembert equation for $(L, C_K, C_V)$ is trivial. The constraint equations are the only relevant equations. They give precisely \(24\) and \(23\). As a consequence, we can describe the thermo-mechanical system presented in Section 2.2.3 as a SOCS [see Remark 3].

3.3.3 Another thermodynamic potentials

An alternative description of the previous thermo-mechanical system can be given by considering the Helmholtz free energy $H := U - TS$ when defining the Lagrangian function. In other words, let us consider $Q$ as above, but define
\[
L \left( x, P, T, V, S, U, \dot{x}, \dot{P}, \dot{T}, \dot{V}, \dot{S}, \dot{U} \right) := \frac{m \dot{x}^2}{2} - mgx - U + TS.
\]

Also, define $C_K$ by \(44\) and \(47\), and $C_V$ by \(46\) and \(48\). Now, the generalized Lagrange-D’Alembert equation, together with the constraints $T = T_0$ and $Ax = V$, give exactly the Eq. \(24\). The Eqs. \(23\) are obtained from \(44\) and \(47\). We can say that it is more natural to use $H$ instead of $U$ in order to define the present thermo-mechanical system as a SOCS, in the sense that, under such a choice, the variational condition turns out to be non trivial. Nevertheless, the only thermodynamical potential that we shall consider from now on (to construct the Lagrangian functions) will be the internal energy.

3.3.4 Vertical piston with dissipation

Let $Q = \mathbb{R} \times \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}$, denote by $(x, P, T, V, S, U; T_c, S_c, U_c)$ the points of $Q$ and define $L : TQ \to \mathbb{R}$ as
\[
L \left( x, P, T, V, S, U, T_c, S_c, U_c, \dot{x}, \dot{P}, \dot{T}, \dot{V}, \dot{S}, \dot{U}; T_c, S_c, U_c \right) = \frac{m \dot{x}^2}{2} - mgx - U - U_c,
\]
with \( m \) and \( g \) positive constants. Consider the submanifold \( C_K \subset T^{(2)}Q \) given by the equations (44) plus

\[
S = S_0 + N_0 R \ln \left( \frac{T^0 V}{T_0 V_0} \right), \quad U_c = \nu T_c, \quad S_c = \nu \ln \left( \frac{T_c}{T_{c,0}} \right) + S_{c,0}
\]

and [see (33) and (34)]

\[
\dot{E}_{mec} + \dot{U}_c = -\kappa A (T - T_c) \quad \text{and} \quad \dot{E}_{mec} + \dot{U} + \dot{U}_c = 0.
\]

On the other hand, take \( C_V \subset TQ \times_Q TQ \) given by Eqs. (46) plus

\[
\delta S = N_0 R \left( \frac{\delta V}{V} + \alpha \frac{\delta T}{T} \right), \quad \delta U_c - \nu \delta T_c = 0, \quad \delta S_c = \nu \left( \frac{\delta T_c}{T_c} \right),
\]

\[
\delta U = -P \delta V \quad \text{and} \quad \delta U_c = \mu \dot{x} \delta x,
\]

where \( N_0, R, \alpha, S_0, S_{c,0}, T_0, T_{c,0}, V_0, k, A, \mu \) and \( \nu \) are positive constants, and \( A \) is the area through which heat flows.

The generalized Lagrange-D’Alembert equation for \((L, C_K, C_V)\) is

\[
-m \ddot{x} \delta x - mg \delta x - \delta U - \delta U_c = 0.
\]

Using the variational constraints in Eqs (46) and (49) it is easy to show that the equation above reduces to the Newton’s Eq. (30). So this equation together with the kinematic constraints defined above are exactly the Equations involved in the thermo-mechanical system presented in Section 2.3, and then the vertical piston with dissipation is also a SOCS.

As for the wagon in a thermal bath, if we do not assume the Fourier’s law, we have again a SOCS for which, in addition, the Second Law must be requested (because it is not automatically satisfied).

Completing this description, let us note again that the manifold \( Q \) can be written as a Cartesian product of \( \mathcal{M} = \mathbb{R} \) and \( \mathcal{T} = \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}^+ \). Nonetheless, the latter can also be decomposed as a product of two contact manifolds \( \mathcal{T}_1 \) and \( \mathcal{T}_2 \), i.e. this is a composite system [see Remark I], where \( \mathcal{T}_1 = \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+ \) represents the ideal gas and \( \mathcal{T}_2 = \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R} \) represents the container, and the contact form is given by \( \theta = dU - TdS + PdV + dU_c - T_c dS_c \) [see Remark I].

3.4 Variational formulation of thermo-mechanical systems

Taking into account the previous examples (and our knowledge of mechanical and thermodynamic systems -see Appendix-), we shall develop a proposal to describe the thermo-mechanical systems as SOCSs. In order to do that, let us summarize what the above SOCSs \((L, C_K, C_V)\) have in common.

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3.4.1 The configuration space

The manifold $Q$ can be written as a Cartesian product $Q = M \times T$, where $M$ and $T$ are manifolds that define the mechanical and the thermodynamic observables, respectively. Also, $T$ is an open subset of $\mathbb{R}^{2d+1}$, for some $d \in \mathbb{N}$, and, consequently, $T$ is a contact manifold. Moreover, $T$ has a distinguished set of global coordinates. As in the Appendix, let us denote the latter by $(x_1, ..., x_{d-1}, T, y_1, ..., y_{d-1}, S, U)$. (50)

3.4.2 The Lagrangian function

The Lagrangian $L : TQ \rightarrow \mathbb{R}$, identifying $T(M \times T)$ with $T^*M \times TT$, can be written as a sum

$$L(a, b) = L_{mec}(a) - U(\tau(b)), \quad \forall a \in TM, \ b \in TT,$$

for some function $L_{mec} : TM \rightarrow \mathbb{R}$. Here, $\tau : TT \rightarrow T$ is the canonical projection. For instance, for the vertical piston of Section 2.2, we have $M = \mathbb{R}$ and $L_{mec} : T\mathbb{R} \rightarrow \mathbb{R}$ such that

$$L_{mec}(x, \dot{x}) = \frac{m\dot{x}^2}{2} - mgx.$$

Remark. Note that the energy $E : TM \times TT \rightarrow \mathbb{R}$ of $L$ is

$$E(a, b) = E_{mec}(a) + U(\tau(b)),$$

being $E_{mec} : TM \rightarrow \mathbb{R}$ the energy of $L_{mec}$. For instance, for the vertical piston,

$$E_{mec}(x, \dot{x}) = \frac{m\dot{x}^2}{2} + mgx.$$

3.4.3 Kinematic constraints

Identifying $T^{(2)}Q$ and $T^{(2)}M \times T^{(2)}T$, the kinematic constraints always satisfy

$$C_K \subset (T^{(2)}M \times T^{(2)}N) \cap C_{E, dQ},$$

where $N \subset T$ is a Legendre submanifold related to the (thermodynamic) state equations (see Remarks [1] and [3]) and $C_{E, dQ}$ is defined as follows.

Consider the canonical projections $\tau^{(1,2)} : T^{(2)}Q \rightarrow TQ$ and $\tau^{(2)} : T^{(2)}Q \rightarrow Q$, and the canonical immersion $j^{(2)} : T^{(2)}Q \rightarrow TTQ$. Finally, define $C_{E, dQ}$ as the submanifold given by the points $\eta \in T^{(2)}Q$ such that

$$\langle dE(\tau^{(1,2)}(\eta)), j^{(2)}(\eta) \rangle = \langle dQ(\tau^{(2)}(\eta)), \tau^{(1,2)}(\eta) \rangle, \quad (51)$$

Recall that, given a Lagrangian function $L : TQ \rightarrow \mathbb{R}$, its energy $E : TQ \rightarrow \mathbb{R}$ is given by

$$E(v) = (FL(v), v) - L(v), \quad \forall v \in TQ,$$

being $FL : TQ \rightarrow T^*Q$ the fiber derivative of $L$, i.e. the Legendre transformation related to $L$.

The local representative of $j^{(2)}$ (in the above mentioned local charts) is

$$j^{(2)}(q, \dot{q}, \ddot{q}) = (q, \dot{q}, \dot{q}, \ddot{q}).$$
being $E$ the energy of $L$ and $dQ$ a 1-form on $Q$. It would be enough to take $dQ$ as a 1-form on $\mathcal{N}$. We take it this way just for simplicity.

Eq. (51) is a second order constraint corresponding to the energy conservation assumption $ECP$ (see Section 2.2.4), where $dQ$ represents the infinitesimal heat exchange between the system and the environment. For instance, for the wagon with internal friction in a thermal bath (see Section 2.1.2),

$$C_{E, dQ} = \left\{ (x, T, S, U, \dot{x}, \dot{T}, \dot{S}, \dot{\bar{U}}) : m \ddot{x} + \dot{U} = \kappa (T_b - T) \right\}.$$

Depending on the system, beside those defined by $\mathcal{N}$ and $C_{E, dQ}$, additional constraints use to be present.

For instance, for all the versions of the vertical piston we have the geometrical constraint $Ax = V$, which defines a submanifold $C \subset T^{(2)}\mathcal{M} \times T^{(2)}\mathcal{T}$. For the adiabatic version we have the constraint $PV^{\gamma} = k$, and for the version with dissipation (see Section 2.3) we have

$$\dot{T} = \frac{\kappa A}{\alpha N_0 R} (T_e - T),$$

corresponding to the Fourier’s law. The last two constraints only involve thermodynamic observables, and define submanifolds $C_{ter}^K \subset T^{(2)}\mathcal{N}$. In the examples given in this paper there are no constraints on the mechanical observables alone. Constraints of this kind would define a submanifold $C_{mec}^K \subset T^{(2)}\mathcal{M}$. Thus, in general, we can say that $C_K$ is of the form

$$C_K = C \cap (C_{mec}^K \times C_{ter}^K) \cap C_{E, dQ}.$$

### 3.4.4 Variational constraints

On one hand, related to the thermodynamic observables only, each state equation gives rise, by derivation, to a variational constraint. For instance, the ideal gas equation $PV = N_0 RT$ gives rise to the variational constraint

$$\delta PV + P \delta V = N_0 R \delta T.$$

This is why for each $q = (m, n) \in \mathcal{M} \times \mathcal{T}$ and $v \in T_q\mathcal{Q} = T_m\mathcal{M} \times T_n\mathcal{T}$, we have that

$$C_V(v) \subset T_m\mathcal{M} \times T_n\mathcal{N}$$

On the other hand, consider a fiber-preserving map $F : TQ \to T^*Q$ such that

$$\langle F(v), (a, b) \rangle := \langle i^*_\tau(v)F(v), a \rangle + \delta U, \quad \forall (a, b) \in T\mathcal{M} \times T\mathcal{T},$$

where

$$b = (\delta x_1, \ldots, \delta x_{d-1}, \delta T, \delta y_1, \ldots, \delta y_{d-1}, \delta S, \delta U) \in T\mathcal{T},$$

and $i_n : \mathcal{M} \to Q : m \mapsto (m, n)$. Now, define

$$C_F := \{ (v, w) \in TQ \times_T TQ : \langle F(v), w \rangle = 0 \},$$

and [recall Eq. (36)]

$$C_F(v) = C_F \cap \{ v \} \times T_{\tau(v)}\mathcal{Q},$$
for each $v \in TQ$. For the wagon with internal friction, the variational constraint 
$-\mu \dot{x} \delta x + \delta U = 0$ can be described by the subset $C_F$ with (under usual identifications)

$$\mathcal{F} : (x, T, S, U, \dot{x}, \dot{T}, \dot{S}, \dot{U}) \mapsto (x, T, S, U, -\mu \dot{x}, 0, 0, 1).$$

(55)

For the adiabatic vertical piston, the subset $C_F$ with

$$\mathcal{F} : (x, P, T, V, S, U, \dot{x}, \dot{P}, \dot{T}, \dot{V}, \dot{S}, \dot{U}) \mapsto (x, P, T, V, S, U, P_A, 0, 0, 0, 0, 1)$$

describes the variational constraint $P_A \delta x + \delta U = 0$. Note that $\mathcal{F}$ describe the external 
force acting on the underlying mechanical system. It can be shown that

$$C_V(v) \subset (T_mM \times T_nN) \cap C_F(v)$$

in all of the above examples, for some function $\mathcal{F}$. Of course, additional variational 
constraints are usually present, but they depend on each particular system.

### 3.4.5 The Second Law condition

As we said at the end of Section 3.3.4, among all the trajectories

$$\gamma : t \mapsto \gamma(t) = (m(t), n(t)) \in M \times N \subset Q,$$

we have to choose those for which the Second Law holds (unless such a law is automatically 
satisfied). This would mean to impose the additional condition [see Eqs. (68) and (69)]

$$\langle dS(n(t)), \dot{n}(t) \rangle \geq \left\langle \frac{dQ(\gamma(t))}{T(n(t))}, (0, \dot{n}(t)) \right\rangle.$$

(56)

### 3.4.6 Thermo-mechanical systems as SOCSs

Now, we can give a definition of a thermo-mechanical system in terms of SOCSs.

**Definition 3.3.** We shall say that a SOCS $(L, C_K, C_V)$ on $Q$ is a thermo-mechanical system if:

- There exist manifolds $M$ and $T$ such that $Q = M \times T$, being $T$ an open submanifold 
of $\mathbb{R}^{2d+1}$, for some $d \in \mathbb{N}$, with distinguished global coordinates. We shall denote 
the latter as in Eq. (50).

- There exists a function $L_{mec} : T\mathcal{M} \to \mathbb{R}$ such that, using the projections $p^{M,T} : Q \to M, T$ and $\tau : T\mathcal{T} \to T$,

$$L = L_{mec} \circ p^M - U \circ \tau \circ p^T.$$

- There exists a Legendre submanifold $N \subset T\mathcal{T}$, w.r.t. the contact form

$$\theta := dU - T dS + \sum_{i=1}^{d-1} x_i dy_i,$$

and a 1-form $dQ \in \Omega^1(Q)$ such that

$$C_K \subset (T^{(2)}M \times T^{(2)}N) \cap C_E, dQ,$$

where $E$ is the energy of $L$ and $C_E, dQ$ is given by Eq. (51).
For each \( q = (m, n) \in \mathcal{M} \times \mathcal{T} \) and \( v \in T_m \mathcal{M} \times T_n \mathcal{T} \),
\[
C_V(v) \subset (T_m \mathcal{M} \times T_n \mathcal{N}) \cap C_F(v),
\]
where \( C_F(v) \) is given by Eqs. (52), (53), and (54).
The trajectories of \((L, C_K, C_V)\) are those of Definition 3.1 that also fulfill the condition (56).

As an example, we shall consider the dissipative vertical piston as already presented, but now immersed in a thermal bath of constant temperature \( T_b \).

Let \( \mathcal{M} = \mathbb{R}^+ \) and \( \mathcal{T} = \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R} \times \mathbb{R} \times \mathbb{R} \). Denote
\[
(x, P, T, V, S, U; T_c, S_c, U_c)
\]
to the points in \( Q = \mathcal{M} \times \mathcal{T} \). As already shown at the end of Subsection 3.3.4, \( \mathcal{T} \) can be decomposed as a product of two manifolds \((\mathcal{T} = \mathcal{T}_1 \times \mathcal{T}_2)\), where \((x, P, T, V, S, U)\) and \((T_c, S_c, U_c)\) are the global Darboux coordinates of \( \mathcal{T}_1 \) and \( \mathcal{T}_2 \), respectively.

Take \( L_{\text{mec}} = \frac{m \dot{x}^2}{2} - mgx, U_{\text{tot}} = U + U_c \) and define
\[
L = L_{\text{mec}} - U_{\text{tot}}
\]
Labeling \( \theta \) and \( \theta_c \) to the contact forms of \( \mathcal{T}_1 \) and \( \mathcal{T}_2 \) respectively, the contact form of \( \mathcal{T} \), according to Eq. (58), is given by \( \theta_{\text{tot}} = \theta + \theta_c \). The Legendre submanifold \( \mathcal{N} \subset \mathcal{T} \) w.r.t \( \theta_{\text{tot}} \) is given by the state equations of the ideal gas
\[
PV = N_0 RT, \quad U = \alpha N_0 RT, \quad S = S_0 + N_0 R \ln \left( \frac{T^0 V}{T^0_0 V_0} \right),
\]
and the state equations of the container
\[
U_c = \nu_c T_c, \quad S_c = \nu_c \ln \left( \frac{T_c}{T_{c,0}} \right) + S_{c,0}.
\]
The constraint \( C_{E, aQ} \) associated with the \textbf{ECP} is resumed in the equation
\[
m \dddot{x} + m g \dot{x} + \dot{U} + \dot{U}_c = \kappa \nu A_e (T_b - T_c),
\]
where \( \kappa \nu \) is the conduction coefficient between the container and the bath, and \( A_e \) is the area through which heat flows from the container to the bath. Both are being considered as constants.
The additional constraints that completes the description of \( C_K \) are given by the geometrical configuration and the Fourier’s law:
\[
Ax = V \quad \text{and} \quad \dot{U} = -\kappa_i A_i (T - T_c),
\]
where \( \kappa_i \) is the constant conduction coefficient between the gas and the contained. The term \( A_i \) is the area through which heat flows from the gas to the container, which depends linearly on \( x \).
If we take the same variational constraints as in Section 3.3.4, \( C_F \) (under usual identifications) is given by

\[
F : \left( x, P, T, V, S, U; T_c, S_c, U_c, \dot{x}, \dot{P}, \dot{T}, \dot{V}, \dot{S}, \dot{U}; T_c, S_c, U_c \right)
\]

\[
(x, P, T, V, S, U; T_c, S_c, U_c, -\mu \dot{x} + PA, 0, 0, 0, 0, 1; 0, 0, 1)
\]

Finally, the trajectories that do not satisfy the inequality (56) must be discarded.

4 Conclusions and future work

In this paper, we have studied a class of physical systems that combine (a finite number of) mechanical and thermodynamical degrees of freedom: the thermo-mechanical systems. We have taken a special care in deducing the evolution equations of the involved observables, for which we only used the Newton's Law and the First Law of Thermodynamics. These evolution equations have been studied in detail in several examples. Also, observing that such equations are similar to the equations of motion of a constrained mechanical system, we proposed a description of the thermo-mechanical systems in terms of Lagrangian systems with second order constraints: the SOCSs. Moreover, we characterized the manifolds in which such SOCS are defined as Cartesian products of two manifold: one of them is related to the mechanical degrees of freedom, and the other to the thermodynamical ones. The latter, in turn, is a contact manifold \( \mathcal{T} \) with a distinguished contact form. Let us also mention that the kinematical constraints, related to the state equations of the thermodynamical counterpart, define a Legendre submanifold of \( \mathcal{T} \).

In a forthcoming paper, we shall give another description of the thermo-mechanical systems, combining the formulation of thermodynamics present in [18, 17], in terms of Legendre submanifolds, and formulation of mechanics shown in [20, 21, 22], in terms of Lagrangian submanifolds.

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Appendix: Brief background on thermodynamics

Below, we introduce the basic notation and terminology on thermodynamics that we shall use along all of the paper, and recall some fundamental concepts on the subject (see [16, 11, 19, 6]).

* A thermodynamic system is typically defined by \( 2d + 1 \) observables, which we shall denote \( x_1, ..., x_{d-1}, T, y_1, ..., y_{d-1}, S \) and \( U \). The \( x_i \)'s and \( T \) (resp. \( y_i \)'s, \( S \) and \( U \)) are called intensive (resp. extensive) variables. The extensive variables depend on the “size” of the
system, while the intensive ones do not. \( U \) is the \textit{internal energy}, \( T \) is the \textit{temperature} and \( S \) the \textit{entropy}. For example, consider a mixture of \( r \in \mathbb{N} \) different chemical components. In this case, we have that:

- \( d = r + 2 \);
- for \( i = 1, \ldots, r \), each variable \( y_i := N_i \) (resp. \( -x_i := \mu_i \)) represents the number of moles (resp. the chemical potential) of a given type;
- \( x_{r+1} =: P \) is the pressure and \( y_{r+1} =: V \) the volume.

**Remark I.** Sometimes, systems can be seen as composed by “simpler” ones, i.e. those defined by a smaller number of variables. We say in this case that such a system is a composite system. In the last example, each chemical compound can be seen as a part of a composite system.

- The possible values of the variables \( x_1, \ldots, x_{d-1}, T, y_1, \ldots, y_{d-1}, S, U \) give rise to an open manifold \( \mathcal{T} \subset \mathbb{R}^{2d+1} \) (that we shall assume open), usually called the thermodynamical phase space (TPS): the set of states of the system. We can see these variables as coordinates for \( \mathcal{T} \).

\[ \theta := dU - T \, dS + \sum_{i=1}^{d-1} x_i \, dy_i. \]  

Thus, \((x_1, \ldots, x_{d-1}, -T, y_1, \ldots, y_{d-1}, S, U)\) defines a global Darboux system for \((\mathcal{T}, \theta)\), see [4, 18].

**Remark II.** For a composite system (see Remark I) formed out by two simple ones, the TPS is a product manifold \( \mathcal{T} = \mathcal{T}_1 \times \mathcal{T}_2 \) with contact form

\[ \theta := dU_1 - T_1 \, dS_1 + dU_2 - T_2 \, dS_2 + \sum_{i=1}^{d_1-1} x_{1,i} \, dy_{1,i} + \sum_{i=1}^{d_2-1} x_{2,j} \, dy_{2,j}. \]

Here \((x_{k,1}, \ldots, x_{k,d_1-1}, -T_k, y_{k,1}, \ldots, y_{k,d_1-1}, S_k, U_k)\), with \( k = 1, 2 \), are the global Darboux coordinates of \( \mathcal{T}_1 \) and \( \mathcal{T}_2 \).

- By \textit{process} we shall mean every curve \( \Gamma : [a, b] \to \mathcal{T} \). It represents a “continuum” of actions on the system that produce a “continuum” of changes on its states.

- Among the states, a special role is played by a subset \( \mathcal{N} \subset \mathcal{T} \), known as the space of equilibrium states, which is defined by the following two conditions on \( U \). The first one says that, on the equilibrium states, \( U \) and the rest of the extensive variables \( y_i \)’s and \( S \) must be related by the formula

\[ U = \Phi (y_1, \ldots, y_{d-1}, S), \]  

for some function \( \Phi \) (typically homogeneous of degree one). Equation above is known as the Fundamental Equation of the system. The second condition says that, for any
differentiable curve $\Gamma : [a, b] \to \mathcal{N} \subset \mathcal{T}$, the variation $\Delta U := U(\Gamma(b)) - U(\Gamma(a))$ must satisfies

$$\Delta U = Q - W,$$

where $Q = Q(\Gamma)$ and $W = W(\Gamma)$ are the heat and the mechanical work, respectively, interchanged by the system and the environment along the process $\Gamma$. This is the First Law of Thermodynamics.

Remark. When $Q = 0$ along a process, one says that such a process is adiabatic.

At a differential level, Eq. (60) translates to

$$dU = dQ - dW.$$  

Here, $dQ$ and $dW$ are 1-forms on $\mathcal{T}$ such that, given a process $\Gamma$,

$$Q(\Gamma) = \int_{\Gamma} dQ = \int_{a}^{b} \left( dQ(\Gamma(t)) , \frac{d}{dt} \Gamma(t) \right) dt.$$ Idem for $dW$. For instance, for a mixture of chemical components (see above), $dQ$ and $dW$ are given by

$$dQ = T \, dS \quad \text{and} \quad dW = P \, dV + \sum_{i=1}^{r} x_i \, dy_i,$$

at least for some processes. Accordingly,

$$dU = T \, dS - \sum_{i=1}^{r} x_i \, dy_i.$$ In general, we must have

$$dU = T \, dS - \sum_{i=1}^{d-1} x_i \, dy_i.$$ Combining Eqs. (59) and (62), it follows that the subset $\mathcal{N}$ is defined by the equations

$$x_i = - \frac{\partial \Phi}{\partial y_i}(y_1, ..., y_{d-1}, S), \quad T = \frac{\partial \Phi}{\partial S}(y_1, ..., y_{d-1}, S) \quad \text{and} \quad U = \Phi(y_1, ..., y_{d-1}, S),$$

known as state equations. This means that $\mathcal{N}$ is a Legendre submanifold of $(\mathcal{T}, \theta)$ (see [4, 18]).

Remark III. As explained in [11], the function $\Phi$ or, equivalently, the internal energy $U$, is defined by the allowed mechanical work on the system. In other words, $U$ is completely determined if we know the work done $W(\Gamma)$ along any process $\Gamma$. (This information, in fact, not only determines $U$, but also $Q$).

* For instance, the fundamental equation of the so-called ideal gas, with only one chemical component, is given by

$$\Phi(N, S, V) = N \, u_0 \left( \frac{N \, v_0 \, e^{\frac{S - N}{R \, N}}}{V} \right)^{\frac{1}{\gamma}},$$

28
where $\alpha$ is a dimensionless constant, $R$ is the universal constant of ideal gases, and $s_0$, $v_0$ and $u_0$ are constants with units of entropy, volume and energy per mole, respectively (see \[6\] for more details). Thus, the related state equations read

$$\mu = \frac{U}{N} \left( 1 + \frac{1}{\alpha} \left( 1 - \frac{S}{NR} \right) \right), \quad T = \frac{U}{NR\alpha}, \quad P = \frac{U}{V\alpha},$$

(65)

with

$$U = Nu_0 \left( \frac{N v_0 \ e^{\frac{s - s_0}{NR}}}{V} \right)^{\frac{1}{\alpha}}.$$

(66)

Let us mention that the last two equations in (65) and the Eq. (66) are usually written as

$$U = \alpha NRT, \quad PV = NRT \quad \text{and} \quad S = N s_0 + NR \ln \left( \frac{T^a V}{t_0^3 N v_0} \right),$$

(67)

where $t_0 := u_0 / R\alpha$.

* The differentiable curves along the equilibrium states $\Gamma : [a, b] \to \mathcal{N}$ are usually called quasi-static processes (and we shall take this convention). Note that, along such curves, the state equations (63) are satisfied for every $t \in [a, b]$ (by definition of $\mathcal{N}$).

Remark IV. In practice, in order to have a quasi-static process $\Gamma$, the velocity of $\Gamma$ must be small (w.r.t. certain characteristic lengths and times related to the microscopic properties of the system). That is to say, the action that defines the process must produce changes in the states at a very slow rate. This justifies the name “quasi-static.” However, in this paper, when we say that a process is quasi-static we will not be assuming that the rate of change of states is necessarily slow. We will only assume that the state equations are satisfied for all time along such a process.

* Not every process $\Gamma : [a, b] \to \mathcal{N}$ is allowed. According to the Second Law of Thermodynamics, a process $\Gamma$ must satisfy

$$\Delta S := S(\Gamma(b)) - S(\Gamma(a)) \geq \int_{\Gamma} \frac{d\mathcal{Q}}{T},$$

(68)

where

$$\int_{\Gamma} \frac{d\mathcal{Q}}{T} := \int_a^b \left( d\mathcal{Q}(\Gamma(t)) \cdot \frac{\frac{d}{dt} \Gamma(t)}{T(\Gamma(t))} \right) dt.$$  

(69)

In infinitesimal terms

$$dS \geq \frac{d\mathcal{Q}}{T}.$$  

(70)

For adiabatic processes, since $d\mathcal{Q} = 0$, we must have $\Delta S \geq 0$.

* A process $\Gamma : [a, b] \to \mathcal{N}$ is say to be reversible if there exists another process $\Gamma^{-} : [a, b] \to \mathcal{N}$ such that $\Gamma^{-}(a) = \Gamma(b)$ and $\Gamma^{-}(b) = \Gamma(a)$. Otherwise, $\Gamma$ is say to be irreversible. Then, a process is reversible if and only if the equation

$$\Delta S = \int_{\Gamma} \frac{d\mathcal{Q}}{T}$$

(71)

holds.
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