

# Mechanics and Thermodynamics: A Semantic Problem of Classification

## Contribution to the solution of a controversial issue

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### RESUMO

Um problema mal formulado origina paradoxos. Uma vez formulado, convenientemente, estes paradoxos são facilmente eliminados. Em mecânica, um dos conceitos geralmente considerado fundamental é o da reversibilidade das suas equações. Desta consideração deriva a bem conhecida afirmação de que a mecânica é irreconciliável com a termodinâmica. Propomo-nos mostrar que só aparentemente estes domínios da física são independentes e que falsos pressupostos estão na origem desta dificuldade de interpretação.

### 1 Newton's law $f=ma$ one of the roots of the problem

It is common knowledge how Newton solved the important problem posed by the movement of comets and planets by introducing the well-known equation  $f=ma$  and the law of universal gravitation. This equation is prophetically valid in relativity [1] if written under the form  $f=dp/dt$  where  $p=m_0\gamma v$ ,  $\gamma=(\sqrt{1-\beta^2})$ ,  $\beta=v/c$ ,  $m_0$  and  $v$  being, respectively, the mass and velocity of the body on a given frame, and  $c$  the velocity of light in vacuum. Problems do arise, however, when considering that  $m_0$  may vary [2].

The problem of the relation between mechanics and thermodynamics lies, in the last analysis, as will be seen, in the definition of quantity  $f$ . In the case of gravitation and of the electromagnetic field the criterion followed was shown to be internally consistent and was consecrated by experimental success.

For gravitation or electromagnetic forces, it is also possible to show, through Hamilton formalism, that there exists invariance in relation to symmetry in time.

In fact, Hamilton canonical equations

$$\dot{p}_k = - \frac{\partial H}{\partial q_k}$$

and

$$\dot{q}_k = \frac{\partial H}{\partial p_k}$$

are symmetric in relation to time, since if  $t$  is associated with  $(-t)$  we have

### ABSTRACT

An ill-formulated problem gives rise to paradoxes. However, once concepts are conveniently defined, such false paradoxes are easily eliminated. In mechanics, one of the concepts generally held as fundamental is the reversibility of its equations. Hence, the well-known statement that mechanics is irreconcilable with thermodynamics. We propose to show that only apparently are the two branches independent and that wrong assumptions are at the basis of this misinterpretation.

$$\frac{d}{dt} \rightarrow \frac{d}{d(-t)} = - \frac{d}{dt},$$

$$\dot{q}_k \rightarrow -\dot{q}_k, p_k \rightarrow -p_k, q_k \rightarrow q_k.$$

Then Hamilton equations may be written

$$- \frac{d}{dt} (-p_k) = - \frac{\partial H}{\partial q_k}$$

$$- \frac{d}{dt} q_k = \frac{\partial H}{\partial (-p_k)}$$

it following that

$$\dot{p}_k = - \frac{\partial H}{\partial q_k}$$

and

$$\dot{q}_k = \frac{\partial H}{\partial p_k}.$$

Once we accept the fact that the domain of mechanics is the one of equation  $f=dp/dt$  other forces, besides those previously referred to, must be taken in account [3] which may simply result from the interaction of mass  $m$  with other particles [4]. This is, in fact, what happens, for example, in the movement of a piston confining a gas in a cylinder, or in the movement of a projectile in the air. Nothing, in such situations, is conceptually different, despite the difficulty of a mathematical definition and measurement of  $f$ . Because the piston moves, the value of  $f$  is altered in relation to its value if

it were at rest (Doppler effect), which makes it necessary to calculate  $f$  on the piston frame [5]. That which causes a false paradox to arise is, as we shall see, precisely the fact that the form of  $f$ , resulting from the piston movement, no longer allows a set of equations, like the ones previously referred to, which permit an invariance in relation to symmetry in time.

## 2 The Concepts of Reversibility in Mechanics

Once we introduce Lagrange function  $L$  of an interactive material points system, it is possible, on certain situations, to proceed to simplifications like, for instance, considering two subsystems  $A$  and  $B$  and split Lagrangean  $L$  into  $L_A$  and  $L_B$  [6]. But nothing, in principle, warrants the statement according to which the movement of a mass  $m$  in interaction with a set of particles, whose number is very large, is outside the sphere of the most general principles of physics which may be called mechanical [3,7]. Now these principles allow to conclude that simplifications give rise to a set of differential equations that are not valid the whole time [8]. In such a case subsystem  $A$  may have a dissipative Hamiltonian [9] which only approximately can describe the interaction with subsystem  $B$  and so, both  $f = dp/dt$  and the equations associated the Hamiltonian cease to be symmetric in time, since they are incomplete [9].

What really happens is that a description in terms of dissipative forces or dissipative Hamiltonians is not a complete description [10] but may be an approximate description for most of the time (Boltzmann, in his famous H theorem also introduced the hypothesis of the molecular chaos, obtaining a solution which is not complete) [11]. But in a more restricted sense equations with dissipative forces or dissipative Hamiltonians belong in mechanics (of physics!) in the sense that they are consistent with the general solution which, at least in principle, may be conceptually arrived at through the momentum-energy conservation [5].

Here is then a well-defined problem of reversibility. In fact, in a complete description, although the "system" [12] (for example, the piston in the previously described model) evolves towards an equilibrium point where it may stay for a long time (say  $10^9$  years) in which case it is reasonable to talk about an irreversible transformation (with time moving forward the piston and the gas will take a long time to repass the initial point...), the equations based on the momentum-energy conservation of all the entities constituting the SYSTEM [12] are, nevertheless, reversible. We can say, then, that in a given sense of reversible (sense I associated with the differential equation) the process is irreversible, in a different sense (sense II associated with the momentum-energy conservation) it is reversible or irreversible, depending on whether one is thinking of an unlimited or limited time (sense IIa and IIb), and in a still different sense ((IIc)-symmetry in time) it is reversible.

Paradoxes will obviously and unavoidably arise if presuppositions are not clearly defined.

We shall now see that, to this difficulty, another problem might be added: that of the concept of reversibility in Thermodynamics.

From what has been said it can be seen that the problem of reversibility, whether in senses I or II, is related to the initial conditions [13]. In fact, for most of the initial conditions, the "system" (for example, the piston) evolves according to the trajectory of the differential equation (non reversible I), although for the initial conditions corresponding to the inversion of all the velocities of all the entities constituting the SYSTEM, the trajectory of the "system" is not consistent with the differential equation and returns to the initial position (reversible IIa). Such conditions are therefore extraordinary, although mathematically possible [14,15]. Equations of mechanics may then be considered irreversible in senses I and IIb and reversible in the other senses.

## 3 Clausius Equation – $dU = dW + dQ$ – the other side of the problem. The various meanings of Heat.

Thermodynamics is generally seen as the domain of heat [16] defined through the so-called "First Principle of Thermodynamics" (FPT)  $dU = dW + dQ$  [2].

But this FPT has given rise to irremovable contradictions [2,17,18].

However, no contradictions or misinterpretations will arise if the Energy Conservation Principle (Energy-Entropy Principle) [12] is used between two equilibrium points by introducing quantities work ( $W$ ) and heat ( $\bar{U}$ ) [12,19]:

$$W = \Delta \bar{U} .$$

If  $\bar{U} = U + U_F$ , where  $U$  is the energy of a subsystem in contact with a source of energy  $U_F$

$$W = \Delta U + \Delta U_F$$

and we can then write  $Q = -\Delta U_F$  if

$$\Delta U = W + Q \quad [2] .$$

For the SYSTEM [12]

$$W = \Delta \bar{U}$$

and the SYSTEM is "mechanical" [20], the classification of "mechanical" and "thermodynamic" no longer making sense ( a "thermodynamic system" is a subsystem of a "mechanical system" ! ) [21].

### 3.1 The notion of equilibrium

We can therefore say that a "mechanical System" tends to an equilibrium point (sense I) and, because of this, internal energy is a function of entropy and volume [22]. (Note that the definition of microscopic entropy associated with the maximum of thermodynamic probability only apparently is incompatible with the fact that the piston and the gas go back to the initial point in the phase space, since the value calculated from the maximum of thermodynamic probability only means that, most of the time, the system is to be found in the microstates of this maximum).

We are thus confronted with two apparently contradictory equilibrium notions: a "mechanical" one, associated with the piston movement – the piston attains

equilibrium position when it "stops" at a given time (in fact the piston is always moving but this movement is physically small); the other notion is a "thermodynamic" one, associated with physical parameters which can be measured in the gas and possess a given mean value in a physically short time interval which may be replaced by an instantaneous quantity. This second notion is consistent with the first most of the time, although the mean value obtained for an infinitely long time coincides with the average obtained in short time intervals for most of the time intervals considered. This does not obviously imply that at some time intervals the piston does not leave its rest position ("equilibrium position"). In the mechanical sense previously defined we would say that during such time intervals we would have an off-equilibrium situation but, in a thermodynamic sense such states are equilibrium states - the mean values obtained for the microstates which maximize thermodynamic probability are the same as those obtained for all possible microstates.

We may, therefore, refer to two equilibrium concepts:

I - equilibrium in a restricted sense, related only to the microstates of thermodynamic maximum probability, generally called equilibrium microstates.

II - equilibrium in a broad sense, related to all possible microstates.

In this second sense the non-equilibrium states are, obviously, the transition states between two equilibrium states.

There arises, then, a notion of reversibility associated with  $dS=0$  [22]. Here also, there appears in "thermodynamics" a terminological confusion which results from mixing up two concepts: the reversible transformation concept and the quasi-static transformation concept [21,23].

Once the incompatibility between "mechanical" and "thermodynamic" is proved to be false, there will be no incompatibility between Boltzmann and Poincaré, or between Carnot and Darwin [16,24]. (Note that the idea of irreversibility appears associated with the evolution of the Universe, since only as an abstraction can a SYSTEM be isolated).

Perhaps the only true incompatibility is to be found in wrongly formulated enunciations [22,23]; for without a convenient interpretation, any attempt to solve the "problem of irreversibility" [25] through mathematical simplifications that create asymmetries may only lead to an apparent solution for an ill-formulated problem.

### 3.2 The notions of heat

Considering what has been said, we have, between two equilibrium points

$$W = \Delta \bar{U}$$

If a subsystem of energy  $U$  is assumed to be in contact with a source of energy  $U_F$ ,

$$W = \Delta \bar{U} = \Delta U + \Delta U_F.$$

In an infinitesimal transformation between two physically near equilibrium points

$$dW = d\bar{U} = dU + dU_F.$$

If we write

$$dU = dW + dQ$$

it follows that

$$dQ = -dU_F.$$

In sense I, let us designate internal energy  $U$  as heat I.

It is obvious that, in this sense, heat of system  $\bar{U}$  cannot coincide with  $U$  or  $U_F$  ( $\bar{U} = U + U_F$ ). This being so, the heat exchanged between the subsystem of energy  $U$  and the source of energy  $U_F$  is  $Q = -\Delta U_F$ .

We have, therefore, a second notion of heat - heat in sense II, or exchanged heat which, in a module, is equal to the variation of heat from source  $\Delta U_F$ .

Let us now consider the elementary variation of a function  $U(V,S)$  in an elementary displacement  $dP$ :

$$dU = \langle dU, dP \rangle$$

where  $dU$  is the exterior derivative of  $U$  and  $\langle dU, dP \rangle$  is the contraction of form  $dU$  and vector  $dP$ .

We therefore have

$$dU = \left( \frac{\partial U}{\partial V} \right)_S dV + \left( \frac{\partial U}{\partial S} \right)_V dS.$$

It can be easily demonstrated that

$$\left( \frac{\partial U}{\partial V} \right)_S = -p$$

and

$$\left( \frac{\partial U}{\partial S} \right)_V = T$$

where  $p$  is the pressure and  $T$  Kelvin temperature [26].

Therefore

$$dU = -p dV + T dS.$$

Let  $dU$  be formally divided into two (Pfaffian) quantities

$$dW = -p dV$$

and

$$dQ = T dS.$$

It is obviously possible to call  $dW$  and  $dQ$  respectively (elementary) work and heat. But to prevent any possible confusion with the other concepts I and II, we must explicitly call them heat III and work III.

These quantities,  $dW$  and  $dQ$ , possess no energetic meaning that can be ascribed to them with generality ( $d$  is crossed precisely to indicate that we are not dealing with exact differentials treated with generality).

Like previously (note that  $dW$  is not necessarily equal to  $dW$ )

$$dW = dU + dU_F = dU - dQ.$$

In a reversible transformation  $d\bar{S} = dS + dS_F = 0$  and  $dW = -p dV = dU + dU_F = -p dV + T dS + T dS_F$ .

Therefore

$$dW = -p dV = dW$$

aaand since

$$d\bar{S} = 0 = dS + dS_F$$

$$dS = -dS_F = -\frac{dU_F}{T} = \frac{dQ}{T}$$

Therefore

$$dQ = T dS = \delta Q$$

In conditions of reversibility, quantity III coincides with quantity II.

Also here, it is obvious that if concepts are not clearly defined, contradictions will inevitably arise [17,18].

Bearing in mind what has been said [5], let us now consider the previously mentioned model of a gas whose particles move perpendicularly to a piston in motion without friction with the walls of the cylinder containing the gas.

The pressure exerted on the piston may be written under the form  $p' = p(1 - 2\dot{x}/u)$  where  $\dot{x}$  and  $u$  are the piston and particle velocity components and  $p$  is the pressure when the piston is at rest at height  $x$ , the height of the piston in relation to the bottom of the cylinder.

The work of this dissipative force is, in an infinitesimal transformation,

$$dW_{diss.} = dE$$

where  $E$  represents the sum of the kinetic and potential energies of the piston.

In fact, the work of the conservative force, "piston weight", is

$$dW_{cons.} = -dV$$

where  $V$  is the piston potential energy.

The total work is, therefore,

$$dW = dW_{cons.} + dW_{diss.} = dT$$

where  $T$  is the kinetic energy of the piston.

So,

$$dW_{diss.} = dE = d(T + V)$$

Since

$$dE + dU = 0$$

$U$  being the gas energy, we can also easily write

$$dU = -dE = -dW_{diss.} = -p'dV$$

where

$$p' = p \left( 1 - \frac{2\dot{x}}{u} \right)$$

as previously stated.

If we formally write

$$U = U(V, S)$$

we have

$$dU = -pdV + TdS = -p'dV$$

and therefore

$$TdS = -(p' - p)dV$$

Now

$$dV = dx \cdot A$$

where  $A$  is the piston area.

Therefore

$$T \frac{dS}{dt} = -(p' - p) \dot{x} A \frac{1}{T}$$

it following that

$$\frac{dS}{dt} = -(p' - p) \dot{x} A \frac{1}{T}$$

Whether for  $\dot{x} < 0$  or for  $\dot{x} > 0$ ,  $dS/dt$  is greater than zero.

Let us consider the case where the "gas" is composed of one particle. Here

$$p' = p \left( 1 - \frac{2\dot{x}}{u} \right)$$

It therefore follows that

$$\begin{aligned} \frac{dS}{dt} &= -p \left( -\frac{2\dot{x}}{u} \right) \dot{x} A \frac{1}{T} = \\ &= p \frac{2\dot{x}^2}{u} A \frac{1}{T} \end{aligned}$$

Since

$$p = \frac{NKT}{V} = \frac{NKT}{Ax}$$

$$\frac{dS}{dt} = NK \frac{2\dot{x}^2}{u} \frac{1}{x}$$

assuming that for  $N$  particles the mean force is the same as the one calculated for one particle.

We can thus calculate the "production" of entropy through an expression which is generally associated with reversibility: ( $dU = -p dV + T dS$ ).

#### 4 The Problem of Determinism

It is commonly affirmed that mechanics equations are "deterministic", which is an entirely meaningless statement [27]. In fact, any presuppositions chosen should be clearly defined.

There exist at least two concepts of determinism that must be taken into account: a scientific and a metaphysical one [28].

A certain theory associated with a system would be deterministic in a scientific sense if it allowed a knowledge of the future of that system. To this end it would be necessary to know the future of the Universe, which is obviously out of the question. Scientific determinism is entirely impossible, as the observer himself would have to be included in the Universe.

Metaphysical determinism is linked with the idea that "nature knows itself" and is, in this sense, determined [28].

Now, as already seen, although in very simple situations, "mechanics" equation  $f = dp/dt$  allows the knowledge of the future (two-body problem). But Poincaré has shown that the introduction of a third body suffices to alter the idea that "mechanics" is scientifically determined.

In fact, as we have seen in the simplified model presented, not even  $f = dp/dt$  is exclusively mechanical, since it is not equivalent to the complete solution obtained through momentum-energy; nor is the complete solution scientifically determined, because

even for a finite number of particles the information which would have to be processed in order to know the whole future, would have to be infinite. However, the physical model would be metaphysically determined.

From the previous analysis we can see that the problem associated with differential equations that are sensitive to initial conditions is not the only one that questions the determinism of "mechanics"; for, in fact, a differential equation which tends to an equilibrium point is not a complete solution for metaphysically determined physical model whose rigorous solution, conceivable in principle, cannot be scientifically determined.

## 5 Conclusion

It has been shown that it is possible to reduce "thermodynamics" to "mechanics", which means that both "mechanics" and "thermodynamics" belong to physics!

The apparent impossibility of such a reduction is due to the fact that definitions in the domains of "mechanics" and "thermodynamics" should be conveniently revised: "mechanics" must accept dissipative forces as an approximation, and "thermodynamics" must accept the tendency to equilibrium contained in this approximation as part of the most general solution obtained through the momentum-energy conservation - entropy characterizes that part of energy which has a dissipative character. The Energy-Entropy Principle (E.E.P.) can replace the incorrect formulation of the "First" Principle of Thermodynamics (F.P.T.) and of the "Second" Principle of Thermodynamics (S.P.T.), since the E.E.P. is the Energy Conservation Principle plus the tendency to define a new equilibrium state. The F.P.T. is merely a mathematical formulation which has no general physical meaning, as quantities  $\delta W = -p dV$  and  $\delta Q = T dS$  do not allow an energetic interpretation with generality. The inability to understand this lies mainly in the fact of considering as equivalent two statements contained in two enunciations that only orally are identical:

- I) In a "reversible" transformation, elementary work is  $\delta W = -p dV$  and heat  $\delta Q = T dS$ .
- II) In a reversible transformation, elementary work is  $dW = -p dV$  and heat  $dQ = T dS$ .

In fact, as shown on the diagram in the appendix, in a transformation between two physically near equilibrium points,

$$dW = d\bar{U} = dU + dU_F = dU - dQ,$$

$U_F$  being the energy of a thermal reservoir. Since  $dU = -p dV + T dS$  and  $dU_F = T_F dS_F$ ,  $dW = -p dV + T dS + T_F dS_F$ . In a reversible transformation  $dS + dS_F = 0$  and  $dW = -p dV$ . Therefore  $T = T_F$ . This being so,  $dS_F = -dU_F/T_F = dQ/T$ .

Because

$$d\bar{S} = dS + dS_F \geq 0$$

then

$$dS \geq -dS_F$$

$$dS \geq \frac{dQ}{T}$$

If the transformation is reversible,  $dS = dQ/T$  and  $dW = -p dV$ .

Since by definition  $\delta Q = T dS$ , in a reversible transformation  $dQ = \delta Q$  (only in a reversible transformation does  $\delta Q$  correspond to the heat exchange with the thermal reservoir).

The use of  $dU = \delta W + \delta Q$  as an energy conservation principle [17,29,30] may lead to error, as entities  $\delta W$  and  $\delta Q$  are confused with exchanged energy. The E.E.P. contains the information afforded by the Energy Conservation Principle and by the asymmetry between internal energy and work and it should not therefore be confused with the expression  $dU = \delta W + \delta Q$  whose physical significance can not be generalized.

The various concepts of "work", "heat", "reversible", "equilibrium", "mechanics" and "thermodynamics" originated a false problem whose solution can only be found upon a careful revision of the physical meaning of all the entities involved.

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