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# An alternative formulation of classical mechanics based on an analogy with thermodynamics

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## Abstract

We study new Legendre transforms in classical mechanics and investigate some of their general properties. The behaviour of the new functions is analysed under coordinate transformations. When invariance under different kinds of transformations is considered the new formulation is found to be completely equivalent to the usual Lagrangian formulation, recovering well-established results such as conservation of angular momentum. Furthermore, a natural generalization of the Poisson bracket is found to be inherent to the formalism introduced. On the other hand, we find that with a convenient redefinition of the Lagrangian,  $\mathcal{L}' = -\mathcal{L}$ , it is possible to establish an exact one-to-one mathematical correspondence between the thermodynamic potentials and the new potentials of classical mechanics.

(Some figures may appear in colour only in the online journal)

## 1. Introduction

The Legendre transform is a powerful tool with important applications in virtually every branch of physics. It is not the purpose of this paper to study the nature of the Legendre transform itself. For this the reader is referred to other papers [1–3] that consider the various aspects and subtleties of the Legendre transform with full mathematical rigour. In this paper we deal with new functions in classical mechanics, which we derived by Legendre transforms from the usual Lagrangian and Hamiltonian formulations, employing only the mathematical machinery that is customary in these theories.

As is well known, the Hamiltonian ( $H$ ) can be derived from a regular Lagrangian ( $\mathcal{L}$ ) via a Legendre transform, namely

$$H(q_i, p_i) = \sum_{i=1}^N \dot{q}_i p_i - \mathcal{L}(q_i, \dot{q}_i). \quad (1)$$

It is typically assumed that this transformation is the only Legendre transform that is useful in classical mechanics. However, in thermodynamics we have *four* fundamental functions,

relating the *four* natural variables  $T, P, V, S$ . Each of these functions can be obtained from any of the other three by a Legendre transformation. One naturally wonders what applications the *unused* ‘mechanical potentials’ might have. This paper studies the extension of classical mechanics to one with two additional dynamical potentials that parallel the Gibbs and Helmholtz free energies in thermodynamics, thus completing the couple formed by  $H$  and  $\mathcal{L}$ .

With the introduction of two new functions, we have a set of four ‘mechanical potentials’ obtained by transformations of the ‘four’ dynamical variables  $p_i, q_i, \dot{q}_i, \dot{p}_i$  in exactly the same fashion that the four thermodynamic potentials exchange their dependence upon the natural variables by Legendre transforms. The rest of the paper is organized as follows. In section 2 we introduce *new* Legendre transforms which involve the time derivative of the canonical momentum  $\dot{p}_i$ . In section 3 we analyse these Legendre transforms and derive some results in connection with them. Finally, in section 4 we study the formal mathematical analogies between thermodynamics and classical mechanics.

## 2. Beyond the standard Legendre transform

Here by the *usual* Legendre transform we refer to a transformation that through a regular Lagrangian leads to the Hamiltonian of a classical system, i.e. transformations of the type given by (1). Thus, our aim is to construct functions beyond  $H(q_i, p_i)$  and  $\mathcal{L}(q_i, \dot{q}_i)$  that not only depend on  $q_i, \dot{q}_i$ , and  $p_i$ , but also depend upon  $\dot{p}_i$ . Thus, let us consider the pair of functions

$$J(\dot{q}_i, \dot{p}_i) \quad \text{and} \quad Q(p_i, \dot{p}_i), \quad (2)$$

where

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \quad (3)$$

is the time derivative of the canonical momentum. For reasons that will be clarified later, we consider it convenient to take the Hamiltonian as the starting point for our analysis, in contrast to [4], where we introduced and defined these functions directly from the Lagrangian. Of course, both treatments are compatible and consistent, but it turns out to be more suitable to start from the Hamiltonian to make contact with the thermodynamic structures, as we see in the following sections.

To guarantee that the previously introduced functions are well-defined Legendre transforms, the Hamiltonian  $H(q_i, p_i)$  must be regular not only in the generalized coordinates but in the generalized momentum as well. Once these conditions are satisfied the following transformations can be defined

$$J(\dot{q}_i, \dot{p}_i) = \sum_{i=1}^N (\dot{p}_i q_i - \dot{q}_i p_i) + H(q_i, p_i) \quad (4)$$

$$Q(p_i, \dot{p}_i) = \sum_{i=1}^N \dot{p}_i q_i + H(q_i, p_i). \quad (5)$$

From these definitions it follows that

$$\begin{aligned} dJ &= \sum_{i=1}^N (q_i d\dot{p}_i - p_i d\dot{q}_i) \\ dQ &= \sum_{i=1}^N (q_i d\dot{p}_i + \dot{q}_i dp_i), \end{aligned} \quad (6)$$

which implies

$$\frac{\partial J}{\partial \dot{q}_i} = -p_i \quad \frac{\partial J}{\partial \dot{p}_i} = q_i \quad (7)$$

$$\frac{\partial Q}{\partial \dot{p}_i} = q_i \quad \frac{\partial Q}{\partial p_i} = \dot{q}_i. \quad (8)$$

From equation (8) the following identities, involving the function  $Q(p_i, \dot{p}_i)$ , can be written

$$\frac{\partial Q}{\partial p_i} - \frac{d}{dt} \frac{\partial Q}{\partial \dot{p}_i} = 0. \quad (9)$$

It is interesting to note that they have the same form as Euler–Lagrange equations and will be shown to be useful in the next section.

### 3. Noether's theorem and the symmetry properties of $J$ and $Q$

Noether's theorem states that for any symmetry of the Lagrangian there is a corresponding conserved quantity. In particular, when the Lagrangian does not have an explicit time dependence the usual Legendre transform, the Hamiltonian  $H(q_i, p_i)$ , is constant. We show in detail that this statement holds not only for  $\mathcal{L}(q_i(t), \dot{q}_i(t))$  but also for the functions  $J(\dot{q}_i(t), \dot{p}_i(t))$  and  $Q(p_i(t), \dot{p}_i(t))$  that were introduced in the previous section.

If we evaluate the time derivative of the  $Q$  function

$$\frac{dQ}{dt} = \sum_{i=1}^N \left( \frac{\partial Q}{\partial \dot{p}_i} \ddot{p}_i + \frac{\partial Q}{\partial p_i} \dot{p}_i \right) = \frac{d}{dt} \left( \sum_{i=1}^N \frac{\partial Q}{\partial \dot{p}_i} \dot{p}_i \right) + \sum_{i=1}^N \dot{p}_i \left( \frac{\partial Q}{\partial p_i} - \frac{d}{dt} \frac{\partial Q}{\partial \dot{p}_i} \right). \quad (10)$$

The last term vanishes due to (9) and finally we obtain the following result

$$\frac{d}{dt} \left( Q - \sum_{i=1}^N \frac{\partial Q}{\partial \dot{p}_i} \dot{p}_i \right) = \frac{dH}{dt} = 0, \quad (11)$$

where we have used that,  $Q - \sum_{i=1}^N \frac{\partial Q}{\partial \dot{p}_i} \dot{p}_i = H$ , in accordance with equations (5) and (8). It is worth noting that an identical constraint can be derived making use of the other dynamical function  $J(\dot{q}_i, \dot{p}_i)$ . After some algebra

$$\frac{dJ}{dt} = \sum_{i=1}^N \left( \frac{\partial J}{\partial \dot{q}_i} \ddot{q}_i + \frac{\partial J}{\partial \dot{p}_i} \ddot{p}_i \right) = \sum_{i=1}^N (q_i \ddot{p}_i - p_i \ddot{q}_i) = \frac{d}{dt} \left( \sum_{i=1}^N q_i \dot{p}_i - p_i \dot{q}_i \right). \quad (12)$$

This result automatically implies that

$$\frac{d}{dt} \left( J - \sum_{i=1}^N (q_i \dot{p}_i - p_i \dot{q}_i) \right) = 0. \quad (13)$$

Taking into account the definition of  $J(\dot{q}_i, \dot{p}_i)$  given in (4) the last expression is nothing but the conservation of the Hamiltonian once again.

#### 3.1. Some examples: invariance under rotations and conservation of angular momentum. The harmonic oscillator

Now we are interested in the existence of conserved quantities linked with symmetries of these dynamical functions  $J(\dot{q}_i, \dot{p}_i)$ ,  $Q(p_i, \dot{p}_i)$  that we have introduced, but from a more general point

of view. For instance, let us consider an arbitrary transformation of the  $Q(p_i, \dot{p}_i)$  function. The variation  $\delta Q$  will be equal to

$$\delta Q = \sum_{i=1}^N \left( \frac{\partial Q}{\partial \dot{p}_i} \delta \dot{p}_i + \frac{\partial Q}{\partial p_i} \delta p_i \right). \quad (14)$$

This can be rewritten according to

$$\begin{aligned} \delta Q &= \frac{d}{dt} \left( \sum_{i=1}^N \frac{\partial Q}{\partial \dot{p}_i} \delta p_i \right) - \sum_{i=1}^N \left( \frac{d}{dt} \frac{\partial Q}{\partial \dot{p}_i} \right) \delta p_i + \sum_{i=1}^N \frac{\partial Q}{\partial p_i} \delta p_i \\ &= \frac{d}{dt} \left( \sum_{i=1}^N \frac{\partial Q}{\partial \dot{p}_i} \delta p_i \right) + \sum_{i=1}^N \left( \frac{\partial Q}{\partial p_i} - \frac{d}{dt} \frac{\partial Q}{\partial \dot{p}_i} \right) \delta p_i. \end{aligned} \quad (15)$$

Due to (9) the second term vanishes, and (15) gives the result

$$\delta Q = \frac{d}{dt} \left( \sum_{i=1}^N \frac{\partial Q}{\partial \dot{p}_i} \delta p_i \right). \quad (16)$$

Thus, if the transformation is a symmetry of the function  $Q$  ( $\delta Q = 0$ ), the quantity  $R \equiv \sum_i (\partial Q / \partial \dot{p}_i) \delta p_i = \sum_i q_i \delta p_i$  is a conserved constant of motion. It is worth noting that  $\sum_i q_i \delta p_i$  will have dimensions of angular momenta if the canonical momentum is equal to the linear momentum. Indeed, to better understand the last result, let us consider an arbitrary rotation in three dimensions. Under a rotation of angle  $\theta$  around the  $z$  axis, the components of the momentum transform according to

$$\begin{aligned} \begin{pmatrix} p'_x(\theta) \\ p'_y(\theta) \\ p'_z(\theta) \end{pmatrix} &= \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} \\ p'_x(\theta) &= p_x \cos \theta + p_y \sin \theta \\ p'_y(\theta) &= p_y \cos \theta - p_x \sin \theta. \end{aligned} \quad (17)$$

For an infinitesimal transformation

$$\begin{aligned} \delta p_x &= p_y \\ \delta p_y &= -p_x. \end{aligned} \quad (18)$$

Therefore, if  $Q$  remains invariant under the infinitesimal rotation, we can derive the conservation of the angular momentum directly from (16)

$$\begin{aligned} \frac{d}{dt} \left( \sum_{i=1}^N \frac{\partial Q}{\partial \dot{p}_i} \delta p_i \right) &= \frac{d}{dt} \left( \sum_{i=1}^3 q_i \delta p_i \right) = \frac{d}{dt} (x \delta p_x + y \delta p_y) \\ &= \frac{d}{dt} (x p_y - y p_x) = \frac{d}{dt} (L_z) = 0. \end{aligned} \quad (19)$$

Thus, we have been able to derive results that are identical to those obtained in the Lagrangian picture of classical mechanics. We can establish a one-to-one correspondence to illustrate the main differences between the formulations.

In table 1, ETI denotes explicit time independence. It is very interesting to note the similarities between  $\mathcal{L}$  and  $Q$ . We can say that  $Q$  is a Lagrangian-type function, because it satisfies a particular version of Euler–Lagrange equations (9)

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} &= 0 \\ \frac{\partial Q}{\partial p_i} - \frac{d}{dt} \frac{\partial Q}{\partial \dot{p}_i} &= 0. \end{aligned} \quad (20)$$

**Table 1.** Behaviour under coordinate transformations.

Function	Variables	Transformation	Conserved quantities
$\mathcal{L}$	$q_i, \dot{q}_i$	$q_i \rightarrow q'_i$	$\sum_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \delta q_i$
$Q$	$p_i, \dot{p}_i$	$p_i \rightarrow p'_i$	$\sum_i \frac{\partial Q}{\partial \dot{p}_i} \delta p_i$
$H$	$q_i, p_i$		
$J$	$\dot{q}_i, \dot{p}_i$	ETI	$J - \sum_i (q_i \dot{p}_i - p_i \dot{q}_i)$

In addition, it has very similar invariance properties under coordinate transformations

$$\begin{aligned} \delta \mathcal{L} = 0 &\Rightarrow \sum_{i=1}^N \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \delta q_i = C \\ \delta Q = 0 &\Rightarrow \sum_{i=1}^N \frac{\partial Q}{\partial \dot{p}_i} \delta p_i = C'. \end{aligned} \tag{21}$$

The reason for these mathematical similarities lies in the fact that the functions  $\mathcal{L}$  and  $Q$  differ only by a total derivative. Indeed, using (1) and (5) it is easy to see that

$$\begin{aligned} \mathcal{L}(q_i, \dot{q}_i) &= \sum_{i=1}^N \dot{q}_i p_i - H = \sum_{i=1}^N \dot{q}_i p_i - \left( Q(p_i, \dot{p}_i) - \sum_{i=1}^N \dot{p}_i q_i \right) \\ &= \frac{d}{dt} \left( \sum_{i=1}^N q_i p_i \right) - Q(p_i, \dot{p}_i). \end{aligned} \tag{22}$$

From our point of view, the choice of one formulation or another is only a matter of convenience, because they are dynamically equivalent and lead to the same physical results that we have proved. This is consistent with the known fact [5] that assures the independence of classical mechanics under canonical transformations, which are more general than Legendre transforms.

Having reached this point, we want to apply the theoretical framework developed with the introduction of the mechanical potentials  $Q(p_i, \dot{p}_i)$  and  $J(\dot{q}_i, \dot{p}_i)$  to a practical problem. Let us discuss briefly how they can be successfully applied to the well-known one-dimensional harmonic oscillator. The Hamiltonian is

$$H(x, p) = \frac{p^2}{2m} + \frac{1}{2} kx^2, \tag{23}$$

which provides the well-known identities  $\partial H / \partial p = \dot{x}$ , and  $\partial H / \partial x = kx = -\dot{p} = -f$ . Now, in order to go from  $H(x, p)$  to  $Q(p, \dot{p})$  we should take into account the definition given in equation (5)

$$Q(p, f) = H(x, p) + fx = \frac{p^2}{2m} - \frac{1}{2} fx + fx = \frac{p^2}{2m} + \frac{1}{2} fx = \frac{p^2}{2m} - \frac{f^2}{2k}. \tag{24}$$

At this point, we need to make an important clarification. In this particular case, we have a conservative force that comes directly from a potential, and thus  $Q(p, \dot{p}) \equiv Q(p, f)$ , but in more general situations, where the potential has a dependence on the velocities, this is no longer true. Thus, in this particular case of the harmonic oscillator, we can replace  $\dot{p}$  by

$f$ , and the equations of motion in the  $Q(p, \dot{p})$  picture can be obtained by application of the Euler–Lagrange-type equations (9), particularized to this problem

$$\frac{\partial Q}{\partial p} - \frac{d}{dt} \frac{\partial Q}{\partial f} = 0. \quad (25)$$

This yields

$$p = -\frac{m}{k} \frac{df}{dt}, \quad (26)$$

which looks a bit odd, but if we take the derivative of both sides of the last equation we get

$$\frac{d^2 f}{dt^2} + \frac{k}{m} f = 0. \quad (27)$$

This is exactly the second order differential equation that is expected for an harmonic oscillator of a frequency given by  $\omega^2 = k/m$ .

### 3.2. Generalized Poisson brackets

If it exists, an important concept in classical mechanics is the Poisson Bracket, a binary operation invariant under canonical transformations that governs the time evolution of Hamiltonian mechanics. This concept is defined as follows: given two functions in the phase space,  $f(q_i, p_i)$ ,  $g(q_i, p_i)$ , the Poisson bracket of  $f$ ,  $g$  acquires the form

$$\{f, g\} = \sum_{i=1}^N \left( \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right). \quad (28)$$

This binary operation is antisymmetric:  $\{f, g\} = -\{g, f\}$  and it obeys the Jacobi identity:  $\{f, \{g, h\}\} + \{h, \{f, g\}\} + \{g, \{h, f\}\} = 0$ . Therefore, it is defining a Lie algebra, known as Poisson algebra.

It is worth noting that the Legendre transforms that we introduced in equations (4) and (5) involve a binary operation that can be viewed as a generalization of the Poisson bracket. Indeed, taking into account the partial derivative identities (7), we can write equation (4) as follows:

$$J(\dot{q}_i, \dot{p}_i) = \sum_{i=1}^N (\dot{p}_i q_i - \dot{q}_i p_i) + H(q_i, p_i) = \sum_{i=1}^N \left( \frac{\partial J}{\partial \dot{q}_i} \frac{\partial H}{\partial p_i} - \frac{\partial J}{\partial \dot{p}_i} \frac{\partial H}{\partial q_i} \right) + H(q_i, p_i). \quad (29)$$

In the same fashion, we can find a relation among the two other mechanical potentials  $\mathcal{L}$ ,  $Q$  in terms of another binary operation. Combining equations (22) and (8), we obtain

$$\begin{aligned} \mathcal{L}(q_i, \dot{q}_i) &= \frac{d}{dt} \left( \sum_{i=1}^N q_i p_i \right) - Q(p_i, \dot{p}_i) = \sum_{i=1}^N (\dot{q}_i p_i + q_i \dot{p}_i) - Q(p_i, \dot{p}_i) \\ &= - \sum_{i=1}^N \left( \frac{\partial \mathcal{L}}{\partial q_i} \frac{\partial Q}{\partial \dot{p}_i} - \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \frac{\partial Q}{\partial p_i} \right) - Q(p_i, \dot{p}_i). \end{aligned} \quad (30)$$

The binary operations that appear in these latter equations are very interesting objects, and in some sense can be interpreted as a natural generalization of the usual Poisson bracket. The standard Poisson bracket operates over functions defined in the same space, the phase space of coordinates  $q_i$ ,  $p_i$ . Nevertheless, the binary operators in equations (29) and (30) are connecting functions that live in different spaces. In general, if we have two functions  $f(x_i, y_i)$ ,  $g(z_i, w_i)$  that take values in different spaces characterized by the coordinates:  $x_i, y_i$  and  $z_i, w_i$ , it will be possible to define a generalized Poisson bracket that mixes the functions and their variables

$$\{f(x_i, y_i), g(z_i, w_i)\}^\dagger = \sum_{i=1}^N \left( \frac{\partial f}{\partial x_i} \frac{\partial g}{\partial w_i} - \frac{\partial f}{\partial y_i} \frac{\partial g}{\partial z_i} \right). \quad (31)$$

It is straightforward to verify that the usual Poisson bracket (28) is only a particular case of (31). This identification occurs when the functions are defined in the same space of configurations, the phase space. The reader may verify that if  $x_i = z_i \equiv q_i$ , and  $y_i = w_i \equiv p_i$ , then  $\{f, g\}^\dagger = \{f, g\}$ .

In summary, the compact expressions for (29) and (30) employing the generalized Poisson brackets will be

$$\begin{aligned} J(\dot{q}_i, \dot{p}_i) &= \{J, H\}^\dagger + H(q_i, p_i) \\ \mathcal{L}(q_i, \dot{q}_i) &= -\{\mathcal{L}, Q\}^\dagger - Q(p_i, \dot{p}_i), \end{aligned} \tag{32}$$

where

$$\{J(\dot{q}_i, \dot{p}_i), H(q_i, p_i)\}^\dagger = \sum_{i=1}^N \left( \frac{\partial J}{\partial \dot{q}_i} \frac{\partial H}{\partial p_i} - \frac{\partial J}{\partial \dot{p}_i} \frac{\partial H}{\partial q_i} \right) \tag{33}$$

$$\{\mathcal{L}(q_i, \dot{q}_i), Q(p_i, \dot{p}_i)\}^\dagger = \sum_{i=1}^N \left( \frac{\partial \mathcal{L}}{\partial q_i} \frac{\partial Q}{\partial \dot{p}_i} - \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \frac{\partial Q}{\partial p_i} \right). \tag{34}$$

### 3.3. The variational principle. Physical interpretation of the introduced functions

As is well known, the Lagrangian admits a natural interpretation provided by Hamilton’s principle, which is enough to derive the Euler–Lagrange equations under completely general assumptions. One naturally wonders if the other mechanical potentials could be employed in the same fashion, within the context of some sort of variational principle. Regarding the function  $Q(p_i, \dot{p}_i)$ , we will show that it is possible.

For this purpose, it is convenient to begin with the usual definition of the action integral in terms of the Lagrangian

$$S = \int_{t_1}^{t_2} \mathcal{L}(q_i, \dot{q}_i) dt. \tag{35}$$

Now, making use of equation (22) we can express the action integral in terms of  $Q(p_i, \dot{p}_i)$  and a total derivative

$$\begin{aligned} S &= \int_{t_1}^{t_2} \mathcal{L}(q_i, \dot{q}_i) dt = \int_{t_1}^{t_2} \left( \frac{d}{dt} \left( \sum_{i=1}^N q_i p_i \right) - Q(p_i, \dot{p}_i) \right) dt \\ &= - \int_{t_1}^{t_2} Q(p_i, \dot{p}_i) dt + \left[ \sum_{i=1}^N q_i p_i \right]_{t_1}^{t_2}. \end{aligned} \tag{36}$$

If we compute  $\delta S = 0$  the conditions  $\delta q_i = 0, \delta p_i = 0$  are satisfied by all the allowed trajectories in the extreme points  $t_1, t_2$  and for this reason all the boundary terms will be removed. In particular, the second contribution in (36) vanishes and we get the following expression for the variation of the action integral:

$$\delta S = \int_{t_1}^{t_2} \delta Q(p_i, \dot{p}_i) dt = 0. \tag{37}$$

This means that

$$\delta S = \sum_{i=1}^N \int_{t_1}^{t_2} \left( \frac{\partial Q}{\partial p_i} \delta p_i + \frac{\partial Q}{\partial \dot{p}_i} \delta \dot{p}_i \right) dt = 0. \tag{38}$$



Integrating by parts the last expression

$$\delta S = \left[ \sum_{i=1}^N \frac{\partial Q}{\partial \dot{p}_i} \delta p_i \right]_{t_1}^{t_2} + \sum_{i=1}^N \int_{t_1}^{t_2} \left( \frac{\partial Q}{\partial p_i} - \frac{d}{dt} \frac{\partial Q}{\partial \dot{p}_i} \right) \delta p_i dt = 0 \quad (39)$$

the first is again a boundary term that does not contribute. Finally, the condition of stationary action  $\delta S = 0$  implies for each index  $i$  the following relation

$$\frac{\partial Q}{\partial p_i} - \frac{d}{dt} \frac{\partial Q}{\partial \dot{p}_i} = 0. \quad (40)$$

We have therefore been able to derive the Euler–Lagrange equations for the function  $Q(p_i, \dot{p}_i)$  that we found previously in equation (9) directly from a variational principle. It is worth noting that the equations that satisfy the functions  $\mathcal{L}$  and  $Q$  are symmetric, exchanging the roles of  $q_i$  and  $p_i$ . Thus, the dynamical potential  $Q(p_i, \dot{p}_i)$  can be interpreted as some sort of ‘dual’ function associated to the Lagrangian. It plays the same role as the Lagrangian in the momentum space.

What about the other dynamical potential  $J(\dot{q}_i, \dot{p}_i)$  that was also introduced in the previous sections? Its physical meaning seems more difficult. Nevertheless, we explicitly showed in (13) that it is also possible to obtain in a consistent way the conservation of the Hamiltonian employing this potential. This suggests that this function encodes the same information as any of the other three mechanical potentials, but the dynamical degrees of freedom are organized in a different way. However, this point needs further clarification and will be the subject of future work.

#### 4. A mathematical correspondence between mechanical and thermodynamic functions

The mathematical analogies between classical mechanics and thermodynamics have been studied in several other works [6–10]. In [6], for instance, thermodynamics was formulated in a purely symplectic way, a formulation invariant under general canonical transformations, just as classical mechanics is. It is common to study thermodynamic structures and functions from a symplectic or ‘mechanical’ point of view. However, studying mechanical structures from a point of view parallel to the traditional thermodynamic formalism is less well explored.

Following this latter scheme, it can be demonstrated that Hamilton equations can be written as Maxwell relations [7], which is a remarkable result, but we believe that all the richness of this picture has not yet been completely exploited. Using this ‘thermodynamic approach’ we will establish one-to-one mapping between the different mechanical and thermodynamic Legendre transformations.

With this aim, it is convenient to start the discussion by noting that the internal energy of a thermodynamic system  $\mathcal{U}(S, V)$  has a mathematical structure that resembles the Hamiltonian of a mechanical system. Their differentials are equal to

$$\begin{aligned} d\mathcal{U} &= T dS - P dV \\ dH &= \dot{q} dp - \dot{p} dq. \end{aligned} \quad (41)$$

Indeed,  $PdV$  is just an infinitesimal dynamical work done or received (depending on the sign) by the system. There are situations where  $\dot{p}dq$ , can also be interpreted as an

infinitesimal work. Thus, following this equivalence, it seems natural to establish the one-to-one correspondence

$$\begin{aligned}
 P &\rightarrow \dot{p} \\
 V &\rightarrow q \\
 T &\rightarrow \dot{q} \\
 S &\rightarrow p \\
 \mathcal{U}(S, V) &\rightarrow H(p, q).
 \end{aligned}
 \tag{42}$$

The next step will generate one-to-one mapping between the thermodynamic and mechanical functions by means of Legendre transforms. For example, following (42) to the thermodynamical transformation  $\mathcal{H}(S, P) = \mathcal{U}(S, V) + PV$  will correspond the mechanical  $Q(\dot{p}, p) = H(p, q) + \dot{p}q$ . The  $Q(\dot{p}, p)$  function is well defined in agreement with (5), and has very interesting symmetry properties under different kinds of transformations, as we have studied in detail in the previous section.

In the same way, the so called Gibbs free energy  $\mathcal{G}(T, P) = \mathcal{U}(S, V) - TS + PV$  can be put in direct correspondence with  $J(\dot{p}, \dot{q}) = H(p, q) + \dot{p}q - \dot{q}p$ . This  $J(\dot{p}, \dot{q})$  is exactly the same function defined in (4), and its dynamical behaviour was also analyzed in detail. Finally, we have the transformation,

$$\mathcal{F}(T, V) = \mathcal{U}(S, V) - TS.
 \tag{43}$$

This is the Helmholtz free energy, which following our scheme will map to the mechanical function,

$$\mathcal{L}'(q, \dot{q}) = H(q, p) - \dot{q}p.
 \tag{44}$$

It is straightforward to show that this last function satisfies

$$d\mathcal{L}' = -\dot{p}dq - p d\dot{q}
 \tag{45}$$

and therefore its physical meaning is clear: it represents a redefinition of the Lagrangian,  $\mathcal{L}' = -\mathcal{L}$ .

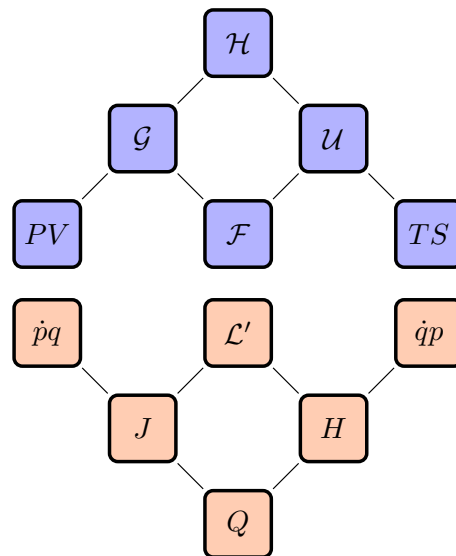
Therefore, the redefinition only implies a global change of sign of the Lagrangian. When we deal with conservative forces we have a change from  $\mathcal{L} = T - V$  to  $\mathcal{L}' = V - T$ . It can be shown that this kind of modification does not have physical consequences, due to the fact that the Euler–Lagrange equations are invariant under the transformation  $\mathcal{L}' \rightarrow -\mathcal{L}$

$$\frac{\partial \mathcal{L}'}{\partial q} - \frac{d}{dt} \frac{\partial \mathcal{L}'}{\partial \dot{q}} = 0.
 \tag{46}$$

It is easy to see that this identity can also be derived using (45). However, although this change of sign is dynamically irrelevant, it allows us to establish an interesting analogy between thermodynamic and mechanical Legendre transformations. Since this is an exact analogy, the relationship is symmetric. We can take any of the dynamical functions  $H(p, q)$ ,  $\mathcal{L}'(q, \dot{q})$ ,  $Q(\dot{p}, p)$ ,  $J(\dot{p}, \dot{q})$  and rebuild by correspondence all the thermodynamic potentials.

In order to make the correspondence more clear and graphic we can use the following Hasse diagrams. In the first Hasse diagram, the ‘magnitude’ of the potentials decreases as you go down the lines.

Thus  $\mathcal{H} = \mathcal{F} + PV + TS$ ,  $\mathcal{G} = \mathcal{F} + PV$ , and  $\mathcal{U} = \mathcal{F} + TS$ . Since the mechanical potentials follow the same pattern they fit perfectly in a similar diagram. In this latter case the ‘magnitude’ increases as you go down the lines:  $Q = \mathcal{L}' + \dot{p}q + \dot{q}p$ ,  $J = \mathcal{L}' + \dot{p}q$ , and  $H = \mathcal{L}' + \dot{q}p$ .



## 5. Concluding remarks

In this paper we have analysed two new Legendre transforms in classical mechanics, the functions  $J(\dot{q}_i, \dot{p}_i)$ ,  $Q(p_i, \dot{p}_i)$ , which involve the time derivative of the canonical momentum, and we have found that they have very interesting and non-trivial symmetry properties under coordinate transformations. In particular, it is remarkable that one of these functions, the so-called  $Q(p_i, \dot{p}_i)$ , can be positioned on equal footing with the Lagrangian of a classical system. On the one hand, it satisfies a particular version of the Euler–Lagrange equations (9). On the other hand, it can also be used successfully to accommodate Noether’s theorem to derive general conservation laws. Therefore, we have introduced here an alternative formulation of classical mechanics that completes the usual picture formed by the Lagrangian ( $\mathcal{L}$ ) and the Hamiltonian ( $H$ ), allowing a broader view of the subject. It is always interesting to show new ways of understanding, demonstrating or deriving familiar results in any physical theory. As Feynman said, ‘Different equivalent descriptions of the same physics are important because they may lead to different ways to extend them’. With the detailed study of the two new mechanical potentials and their properties we were also able to obtain new insights, such as a natural generalization of the Poisson bracket, which was found to be inherent to the formalism introduced. In addition, we realized that a one-to-one correspondence between the different Legendre transformations of classical mechanics and thermodynamics may be established. This can be achieved by paying the price of a dynamically irrelevant (in the case of conservative forces) redefinition of the Lagrangian, from  $\mathcal{L}$  to  $-\mathcal{L}$ . The important thing is to keep the usual definition of the Hamiltonian as  $H = T + V$ . But regarding the Lagrangian in the case of conservative forces, taking the usual definition,  $\mathcal{L} = T - V$  or the alternative  $\mathcal{L}' = V - T$ , is only a matter of choice that has no physical consequences. The fact that the Lagrangian was originally defined as  $\mathcal{L} = T - V$  seems an arbitrary convention established in the absence of more fundamental physical reasons.

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