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Principles of time evolution in classical physics

J Güémez[1,3] and M Fiolhais[2,3]

[1] Department of Applied Physics, Faculty of Sciences, University of Cantabria, Av. de Los Castros, E-39005 Santander, Spain
[2] Physics Department and CFisUC, University of Coimbra, 3004-516 Coimbra, Portugal

E-mail: guemezj@unican.es and tmanuel@uc.pt

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Abstract

We address principles of time evolution in classical mechanical/thermodynamical systems in translational and rotational motion, in three cases: when there is conservation of mechanical energy, when there is energy dissipation and when there is mechanical energy production. In the first case, the time derivative of the Hamiltonian vanishes. In the second one, when dissipative forces are present, the time evolution is governed by the minimum potential energy principle, or, equivalently, maximum increase of the entropy of the universe. Finally, in the third situation, when internal sources of work are available to the system, it evolves in time according to the principle of minimum Gibbs function. We apply the Lagrangian formulation to the systems, dealing with the non-conservative forces using restriction functions such as the Rayleigh dissipative function.

Keywords: Lagrangian, thermodynamics, Rayleigh function

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

1. Introduction

When a system is acted upon only by conservative forces, or when non-conservative forces are present but they do not dissipate energy, it evolves in time with mechanical energy conservation. Newton's second law (for both translations and rotations) is then enough to describe the process, and no thermal effects are present [1]. In section 2, we illustrate this situation by considering a non-slipping disk moving on an incline.

[3] Authors to whom any correspondence should be addressed.

However, in the presence of dissipative forces, the mechanical energy of the system is not conserved and the system evolves according to the principle of minimum potential energy [2]: the endpoint of the trajectory has to be a state of minimum potential energy. In these cases it might be necessary to take into account thermal effects, by using the first law of thermodynamics [3]. The mechanical energy dissipated as heat it taken into account by the first law, and the time evolution of the system follows the principle of maximum entropy: the entropy of the universe increases until it reaches a maximum compatible with the actual conditions of the process (second law of thermodynamics). In section 3, we illustrate this situation by considering a sliding disk on an incline, with both translational and rotational motions, acted upon by a kinetic friction force responsible for the energy dissipation.

Moreover, one may also consider a class of processes for which the system experiences a mechanical energy increase resulting from a non-mechanical source, e.g. chemical reactions. In section 4, we illustrate this case by considering a disk with an internal source of energy, which consists of two cartridges where some chemical reactions take place. The device is able to provide two symmetrical forces that produce a torque on the disk, making it going up an inclined plane. In an ideal process, the maximum work these forces can perform equals the variation of mechanical energy of the disk, and this is still equal to the decrease of the Gibbs' function of the chemical substances [4].

The mechanical study in all three cases is conducted in the framework of the Lagrangian formalism. However, due to the presence of non-conservative forces, it is necessary to complement the formalism using restriction functions. When the non-conservative forces do not perform any work, this can be implemented through the usual Lagrange multipliers. In turn, when the non-conservative forces do work, a Rayleigh dissipation or production function has to be taken into account at the level of the Euler–Lagrange equations. This paper also pedagogically addresses such formalism, which is not very commonly used in the classroom. Our conclusions are summarised in section 5.

2. Evolution with mechanical energy conservation

A disk rolling without slipping on top of an incline, as shown in figure 1, is a common example of a process in which mechanical energy is conserved. For the disk, with radius R and mass m, descending the incline, the Hamiltonian is

$$H(x, p; \theta, J) = \frac{p^2}{2m} + \frac{J^2}{2I} + mg(d - x)\sin\alpha, \tag{1}$$

where x describes the position of the centre-of-mass (initially $x = 0$) along the slope and θ the angular position of the rotating disk (initially $\theta = 0$). The other quantities entering the Hamiltonian have the usual meaning: $p = m\dot{x} = mv$ is the linear momentum, $J = I\dot{\theta} = I\omega$ is the angular momentum, $I = \frac{1}{2}mR^2$ is the moment of inertia, g is the acceleration of gravity, d is the length of the incline and α its inclination angle with respect to the horizontal plane. The non-slipping condition is expressed by the relation between the centre-of-mass velocity and the angular velocity of the disk: $v(t) = \omega(t)R$ or, equivalently, $x(t) = \theta(t)R$. In the Lagrangian formulation, one considers two pairs of variables (x, v) and (θ, ω). In terms of the Lagrangian dynamical variables, the Hamiltonian can be written as

$$H(x, v; \theta, \omega) = \frac{1}{2}mv^2 + \frac{1}{2}I\omega^2 + mg(d - x)\sin\alpha \tag{2}$$

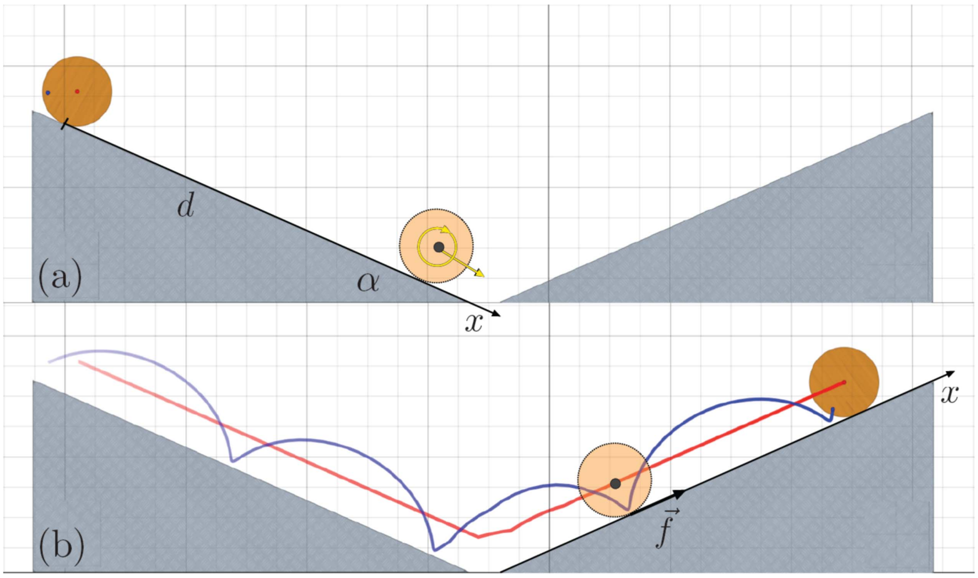

Figure 1. (a) A disk—with a red light spot at its centre and a blue light spot at its rim—rolls down an inclined plane without slipping. In (b) the disc goes up an inclined plane reaching the same vertical level. Simulation performed with the software Algodoo [5].

and then the Lagrangian reads

$$L(x, v; \theta, \omega) = vp + \omega J - H(x, v; \theta, \omega) = \frac{1}{2}mv^2 + \frac{1}{2}I\omega^2 - mg(d - x)\sin\alpha. \quad (3)$$

The Lagrangian formalism is here applied using a restriction function that allows us to explicitly consider the static friction force, $\vec{f}$, exerted by the plane on the rim of the disk [6]. The restriction function implements the interdependence of the variables used in the Lagrangian. The use of restriction functions at the level of the Lagrangian, as we do here, is equivalent to the more familiar addition of a Lagrange multiplier term. When the disk rolls down the incline, the restriction function is given by [7]

$$\mathcal{P}(x, \theta) = -fx + fR\theta = 0, \quad (4)$$

which already takes into account that the force opposes the displacement when the disk descends, making a positive torque that leads to a clockwise increasing angular velocity ($\mathcal{P} \to -\mathcal{P}$ for the disk going up the incline). The Euler–Lagrange equations with such a restriction function are

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial v} - \frac{\partial L}{\partial x} = \frac{\partial \mathcal{P}}{\partial x}, \quad (5)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \omega} - \frac{\partial L}{\partial \theta} = \frac{\partial \mathcal{P}}{\partial \theta}. \quad (6)$$

From here, one obtains, respectively, two equations, namely Newton's second law for the translation and for the rotation, the latter also known as the Poinsot–Euler equation [1]:

$$m\mathrm{d}v - mg\sin\alpha\,\mathrm{d}t = -f\,\mathrm{d}t, \quad (7)$$

$$I\mathrm{d}\omega = \quad fR\ \mathrm{d}t. \tag{8}$$

When the non-slipping condition, which can also be expressed as $\mathrm{d}v = R\mathrm{d}\omega$, is fulfilled, the previous two equations lead to $f = \frac{1}{3}mg\sin\alpha$. This force must be lower than the maximum frictional force, $f^{\max} = \mu_s mg\cos\alpha$, which can be exerted by the plane upon the disk, where μ_s is the coefficient of static friction.

From equations (7) and (8), and using $\mathrm{d}x = v\mathrm{d}t$ and $\mathrm{d}\theta = \omega\mathrm{d}t$, the pseudo-work equations [8] are readily obtained for the translation and rotation,

$$\frac{1}{2}m\mathrm{d}v^2 = (mg\sin\alpha - f)\mathrm{d}x, \tag{9}$$

$$\frac{1}{2}I\mathrm{d}\omega^2 = fR\ \mathrm{d}\theta, \tag{10}$$

which lead to

$$\frac{1}{2}m\mathrm{d}v^2 + \frac{1}{2}I\mathrm{d}\omega^2 = mg\sin\alpha\ \mathrm{d}x. \tag{11}$$

Pseudo-work is defined through the resultant force and the centre-of-mass displacement and it is the part of the work that goes into changing the centre-of-mass kinetic energy [9]. The pseudo-work equation (11) for the process can also be expressed as

$$\mathrm{d}\left[\frac{1}{2}mv^2 + \frac{1}{2}I\omega^2 + mg(d - x)\sin\alpha\right] = 0. \tag{12}$$

One recognises that the quantity in brackets is the Hamiltonian (2) which, of course, is implicitly time dependent through $v(t)$, $\omega(t)$ and $x(t)$. However, equation (12) allows us to conclude that

$$\frac{\mathrm{d}H}{\mathrm{d}t} = 0, \tag{13}$$

and the bottom line is that the mechanical energy is conserved during this process.

The equation expressing the first law of thermodynamics [10] is $\mathrm{d}K_{\mathrm{cm}} + \mathrm{d}U = \delta W + \delta Q$, where the left hand side refers to the centre-of-mass kinetic energy and the internal energy variations, respectively, and the right hand side refers to the work and heat transfers to/from the system during the process. In the present case,

$$\frac{1}{2}m\mathrm{d}v^2 + \frac{1}{2}I\mathrm{d}\omega^2 = mg\sin\alpha\ \mathrm{d}x + \delta Q, \tag{14}$$

where $\delta W = mg\sin\alpha\ \mathrm{d}x$ is just the work performed by the gravitational force, since the other forces do not perform any work. We note that the rotational kinetic energy is disk's internal energy. By comparing equations (12) and (14) one concludes that

$$\frac{\delta Q}{\mathrm{d}t} = 0, \tag{15}$$

i.e. there are no thermal effects during the process. The variation of the entropy of the universe is zero, $\mathrm{d}S_{\mathrm{U}} = -\frac{\delta Q}{T} = 0$, where T is the temperature of the thermal reservoir surrounding the disk. Therefore, the process is reversible and the description of the process is essentially the same whether the disk descends or ascends the inclined plane.

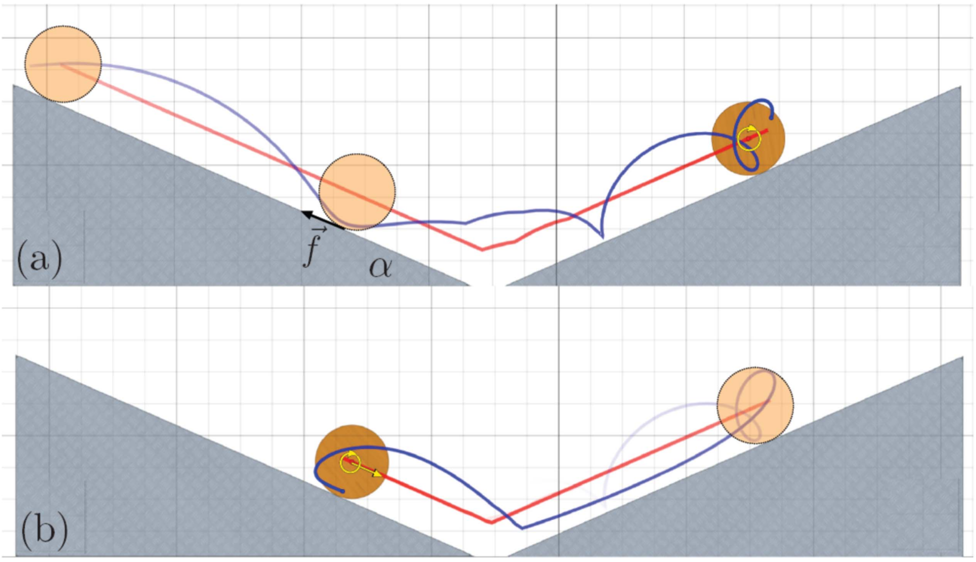

Figure 2. (a) A disk descends an inclined plane, not fulfilling the rolling condition. (b) After damped oscillations in both planes, the disk eventually stops at the bottom of both planes. Simulation performed with Algodoo.

3. Evolution with minimisation of potential energy (maximum entropy)

Next we consider a process in which the disk descends and then ascends the inclined planes, but now one assumes that the static friction coefficient is such that $\mu_s < \frac{1}{3}\text{tg}\,\alpha$. The non-slipping condition is no longer fulfilled and therefore the disk rolls and slides. Figure 2 depicts the process.

The force applied on the rim of the disk is the kinetic friction force, $f^{\text{kin}} = \mu_k mg\cos\alpha$ (μ_k is the coefficient of kinetic friction), and we can still use the pairs of dynamical variables (x, v) and (θ, ω) which are now independent from each other. The Hamiltonian (2) and the Lagrangian (3) are still valid for this process.

The dissipative force is responsible for conversion of mechanical energy into heat, increasing the entropy of the universe [3]. The phenomenological description of this dissipation does not fit naturally into the Lagrangian formalism. However, it can be incorporated in the Euler–Lagrange equation [11], in a heuristic way, through the so-called Rayleigh dissipative function. This Rayleigh function will allow for the correct description of the dynamics of the system. Based on expression (4), for the descendent motion we use the Rayleigh dissipative function $\mathcal{R}(x, \theta) = -f^{\text{kin}}x + f^{\text{kin}}R\theta$ ($\mathcal{R} \to -\mathcal{R}$ for the ascending motion). This function cannot be directly introduced in the Lagrangian, since it would correspond to a potential energy that does not exist [12], so it is introduced at the level of the Euler–Lagrangian equations.

Thus, the two Euler–Lagrange equations are

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial v} - \frac{\partial L}{\partial x} = \frac{\partial \mathcal{R}}{\partial x}, \tag{16}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \omega} - \frac{\partial L}{\partial \theta} = \frac{\partial \mathcal{R}}{\partial \theta}. \tag{17}$$

The translational and rotational equations are now, respectively, given by

$$m\mathrm{d}v - mg\sin\alpha\ \mathrm{d}t = -\mu_{\mathrm{k}} mg\cos\alpha\ \mathrm{d}t, \tag{18}$$

$$I\mathrm{d}\omega = \mu_{\mathrm{k}} mg\cos\alpha\ R\mathrm{d}t. \tag{19}$$

We repeat the process described in the previous section to obtain the pseudo-work equations for translation and for rotation

$$\frac{1}{2}m\mathrm{d}v^2 = (mg\sin\alpha - \mu_{\mathrm{k}} mg\cos\alpha)\mathrm{d}x, \tag{20}$$

$$\frac{1}{2}I\mathrm{d}\omega^2 = \mu_{\mathrm{k}} mg\cos\alpha\ R\ \mathrm{d}\theta, \tag{21}$$

and, after a term by term summation of these two equations, one arrives at

$$\mathrm{d}\left[\frac{1}{2}mv^2 + \frac{1}{2}I\omega^2 + mg(d - x)\sin\alpha\right] = -\mu_{\mathrm{k}} mg\cos\alpha(\mathrm{d}x - R\ \mathrm{d}\theta). \tag{22}$$

So far, we have considered the descendent motion of the disk, but the description of the ascending motion follows the same ideas. From Hamiltonian (2), we can now write, for the sliding disc, for which $v > R\omega$ (whether in the descending or in the ascending motion),

$$\frac{\mathrm{d}H}{\mathrm{d}t} = -\mu_{\mathrm{k}} mg\cos\alpha(v - R\omega). \tag{23}$$

We stress that dissipation always occurs irrespective of the motion being descendant or ascendant. Therefore, the mechanical energy is not conserved in the process: it is dissipated, and concomitantly the value of the Hamiltonian decreases [13]. The disk stops at the position where gravitational potential energy compatible with the process is minimum, i.e. at the bottom of the two inclines.

The first law of thermodynamics equation, assuming that the disk neither varies its temperature nor its entropy, is expressed by [14]

$$\frac{1}{2}m\mathrm{d}v^2 + \frac{1}{2}I\mathrm{d}\omega^2 = mg\sin\alpha\ \mathrm{d}x + \delta Q \tag{24}$$

and comparison with equation (22) allows us to conclude that

$$\frac{\delta Q}{\mathrm{d}t} = -\mu_{\mathrm{k}} mg\cos\alpha\ (v - R\omega) < 0. \tag{25}$$

Thermal effects are present in the process resulting in an increase of the entropy of the universe:

$$\frac{\mathrm{d}S_{\mathrm{U}}}{\mathrm{d}t} = \frac{\mu_{\mathrm{k}} mg\cos\alpha\ (v - R\omega)}{T} > 0 \tag{26}$$

and the process is irreversible.

The expression

$$\frac{\mathrm{d}H}{\mathrm{d}t} = -T\frac{\mathrm{d}S_{\mathrm{U}}}{\mathrm{d}t}, \tag{27}$$

relates the mechanical description of the process with its thermodynamical description [15].

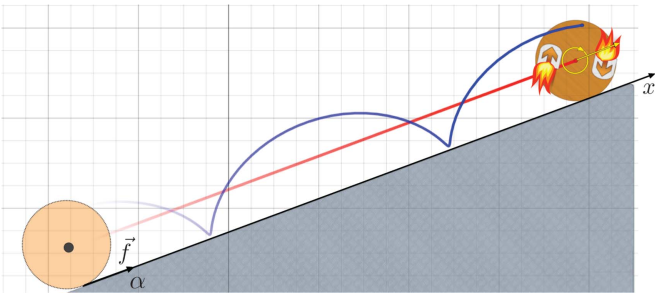

Figure 3. A disk goes up an inclined plane, fulfilling the rolling condition, due to the action of two cartridges where chemical reactions take place. Simulation performed with Algodoo.

4. Evolution with maximum work (minimum of Gibbs function)

Figure 3 shows a disk going up an inclined plane due to two cartridges, where chemical reactions occur, which are fixed close to the rim of the disk in such a way that, while the chemical reactions are taking place, two opposite forces, $\vec{F}$ and $-\vec{F}$, exert a net torque $\tau = 2Fr$ upon the disk (r is the distance from the application point of each force to the centre of the disk). We assume constant F.

The forces exerted on the disk due to the chemical reaction in the cartridges perform work, but it cannot be associated with either a mechanical potential or with a mechanical work reservoir [16] whose potential energy decreases.

The Hamiltonian for this system is

$$H(x, p; \theta, J) = \frac{p^2}{2m} + \frac{J^2}{2I} + mgx \sin\alpha, \tag{28}$$

and the corresponding Lagrangian is

$$L(x, v; \theta, \omega) = \frac{1}{2}mv^2 + \frac{1}{2}I\omega^2 - mgx \sin\alpha. \tag{29}$$

We note that cartridge forces, $\{\vec{F}\}$, produce a positive torque whilst the static friction force, $\vec{f}$, produces a negative torque, $\tau_f = -fR$. We assume that f is lower than the maximum friction force $f^{\max} = \mu_s mg \cos\alpha$, i.e. the non-slipping condition $x = R\theta$ is fulfilled.

In the present case there is mechanical energy production, but we can proceed using a heuristic point of view similar to the one applied in the previous section for the dissipative forces. Now we use a Rayleigh production function $\mathcal{R}_{\mathrm{P}}(x, \theta) = 2Fr\theta$ which should be added to restriction function (4), which, for the ascending motion, reads $\mathcal{P}(x, \theta) = fx - fR\theta = 0$. Altogether, the restriction function turns out to be $\mathcal{P}'(x, \theta) = 2Fr\theta + fx - fR\theta$. Then, the Euler–Lagrange equations for the ascending disk are

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial v} - \frac{\partial L}{\partial x} = \frac{\partial \mathcal{P}'}{\partial x} \rightarrow \frac{\mathrm{d}}{\mathrm{d}t}mv + mg \sin\alpha = f \tag{30}$$

for the translation, and

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \omega} - \frac{\partial L}{\partial \theta} = \frac{\partial \mathcal{P}'}{\partial \theta} \rightarrow \frac{\mathrm{d}}{\mathrm{d}t}I\omega = 2Fr - fR \tag{31}$$

for the rotation. These equations of motion can also be written as

$$m\mathrm{d}v = (f - mg\sin\alpha)\mathrm{d}t, \tag{32}$$

$$I\mathrm{d}\omega = (2Fr - fR)\mathrm{d}t. \tag{33}$$

After some short transient regime, the disk reaches the rolling condition, $v = \omega R$. In this regime, from the above equations, one readily obtains

$$f = \frac{4}{3}F\frac{r}{R} + \frac{1}{3}mg\sin\alpha < \mu_s mg\cos\alpha. \tag{34}$$

Inserting this expression for the static friction force in the equations of motion (32) and (33), and then integrating,

$$v(t) = \left(\frac{4}{3}\frac{F}{m}\frac{r}{R} - \frac{2}{3}g\sin\alpha\right)t, \tag{35}$$

$$\omega(t) = \left(\frac{4}{3}\frac{F}{m}\frac{r}{R^2} - \frac{2}{3}\frac{g}{R}\sin\alpha\right)t. \tag{36}$$

Also from the equations (32) and (33) the pseudo-work equations are obtained:

$$\frac{1}{2}m\mathrm{d}v^2 = \left(\frac{4}{3}F\frac{r}{R} - \frac{2}{3}mg\sin\alpha\right)\mathrm{d}x, \tag{37}$$

$$\frac{1}{2}I\mathrm{d}\omega^2 = \left(\frac{2}{3}Fr - \frac{1}{3}Rmg\sin\alpha\right)\mathrm{d}\theta. \tag{38}$$

Integration leads to

$$v^2(d) = \left(\frac{8}{3}\frac{F}{m}\frac{r}{R} - \frac{4}{3}g\sin\alpha\right)d, \tag{39}$$

$$\omega^2(d) = \left(\frac{8}{3}\frac{F}{m}\frac{r}{R} - \frac{4}{3}g\sin\alpha\right)\frac{1}{R}\theta, \tag{40}$$

hence, the final linear and angular velocities are independent of the coefficient of static friction, provided, of course, the non-slipping condition is fulfilled.

Since $\mathrm{d}x = R\,\mathrm{d}\theta$, from (37) and (38) one has

$$\frac{1}{2}m\mathrm{d}v^2 + \frac{1}{2}I\mathrm{d}\omega^2 + mg\sin\alpha\,\mathrm{d}x = 2Fr\,\mathrm{d}\theta. \tag{41}$$

The mechanical energy variation of the disk is equal to the work performed on the disk by the forces coming from the chemical reactions.

Hence, when the rolling condition is fulfilled,

$$\frac{\mathrm{d}H}{\mathrm{d}t} = 2Fr\omega, \tag{42}$$

expressing the mechanical energy production rate while the reactants are consumed in the cartridges.

To study the thermodynamics of the system, it is convenient to include the cartridges and the reactants (assumed to be massless) in the system. The first law of thermodynamics can then be written as

$$\frac{1}{2}m\mathrm{d}v^2 + \frac{1}{2}I\mathrm{d}\omega^2 + \mathrm{d}U_\xi = -mg\sin\alpha\ \mathrm{d}x - P\mathrm{d}V_\xi + T\mathrm{d}S_\xi, \tag{43}$$

where $\mathrm{d}U_\xi$ is the variation of the chemical internal energy, $-mg\sin\alpha\ \mathrm{d}x$ is the work of the external gravitational force and $-P\mathrm{d}V_\xi$ is the work on the gases produced in the chemical reactions by the external pressure, P, corresponding to a volume variation $\mathrm{d}V_\xi$. The forces $\{\vec{F}\}$ are now internal ones, but internal work does not enter in (43). The rotational kinetic energy is internal energy of the system. Finally, when $\mathrm{d}S_\xi < 0$ in a chemical reaction, a heat transfer to the external thermal reservoir, $\delta Q_{\min} = -T\mathrm{d}S_\xi > 0$, ought to occur in order to ensure that the entropy of the universe does not decrease.

The energy balance equation (43) can still be written as

$$\frac{1}{2}m\mathrm{d}v^2 + \frac{1}{2}I\mathrm{d}\omega^2 + mg\sin\alpha\ \mathrm{d}x = -\mathrm{d}G_\xi, \tag{44}$$

where we have introduced $\mathrm{d}G_\xi = \mathrm{d}U_\xi + P\mathrm{d}V_\xi - T\mathrm{d}S_\xi$, the Gibbs function variation for the chemical reactions.

Comparison with (41) and (42) allows us to write

$$-\frac{\mathrm{d}G_\xi}{\mathrm{d}t} = 2Fr\omega. \tag{45}$$

If the heat transfer to the surrounding is just $\delta Q_{\min}$, the process is reversible (no universe entropy increase) and, at least in principle, the produced mechanical energy can be used back to increase the Gibbs function towards its original value. For instance, if hydrogen and oxygen react producing water, the mechanical energy can be, in principle, totally used to hydrolise the water.

The expression (principle of minimum of Gibbs function),

$$\frac{\mathrm{d}H}{\mathrm{d}t} = -\frac{\mathrm{d}G_\xi}{\mathrm{d}t} > 0, \tag{46}$$

relates the mechanical description with the thermodynamic description of the process. Of course, if the heat transfer is such that $\delta Q > -T\mathrm{d}S_\xi$, then less mechanical energy is obtained than the maximum possible and the process is partly irreversible, with $\mathrm{d}S_\mathrm{U} > 0$. It is completely irreversible if no mechanical energy is obtained and, in this case, $-\mathrm{d}G_\xi = T\mathrm{d}S_\mathrm{U}$.

This process is equivalent to many other processes such as those discussed in [17] and also equivalent to a cyclist riding a bicycle up a mountain slope. In a broad sense, all thermal engines work according to the above mentioned principle.

5. Conclusions

The study of the time evolution of mechanical/thermodynamical systems goes much beyond [18] the analysis that we carried out in this article. Here we have studied three processes that are pedagogically relevant to analyse how classical systems evolve in time and to figure out what is the best evolution criterion to be applied in a concrete situation.

In all cases, we have considered the motion of a disk that rotates while its centre-of-mass also moves, descending or ascending inclined planes. The examples also serve to illustrate how the Lagrangian formalism (used in all three cases) is implemented, even when there are non-conservative forces involved in the processes. Such implementation proceeds via the consideration of the so-called restriction functions, such as the Rayleigh dissipation function when dissipative forces are present.

In the first example, the non-conservative forces do not do any work so the system evolves in a way that the mechanical energy is conserved. In other words, the time derivative of the Hamiltonian of the system is zero. In the second example, we considered the motion of a disk that slides while it rolls and there is dissipation of energy in the surrounding. The system evolves until it reaches the minimum possible potential energy, while the entropy of the universe increases to a maximum value. Finally, in the third example, we show that chemical energy can be transferred without losses to the system, being incorporated as mechanical energy. The time evolution of the system is then governed by the principle of minimum Gibbs function.

A student familiar with the basics of mechanics and thermodynamics may certainly find it useful to compare the three systems studied in this work.

ORCID iDs

M Fiolhais https://orcid.org/0000-0002-6636-9957

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