THERMODYNAMICS AND DYNAMIC SYSTEMS [1]

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Abstract

The aim of this contribution is to attempt to state a thermodynamic theory for dynamic systems modeled by first order differential equation systems. This approach could help us to understand better the nature of complexity if a general definition of Entropy can be defined in the context of these systems. The way followed is stating a Lagrangian-Hamiltonian approach for them. This approach provides a Liouville's equation from which Entropy can be defined. An amazing result arises: for equilibrium distributions, Liouville's function and Entropy depend on system energy. The philosophical conclusion is that a dual deterministic-probabilistic picture of general systems is implicit in their nature, i.e., the probabilistic picture would not arise necessarily from a lower level of description.

Résumé

L'objectif de cette contribution c'est essayer d'établir d'une théorie thermodynamique pour les systèmes dynamiques modélisés par des systèmes d'équations différentielles de premier ordre. Cette approche pourrait nous aider à mieux comprendre la nature de la complexité, si une définition générale d'Entropie peut être définie dans le contexte de ces systèmes. Le chemin suivi est arranger une approche Lagrangienne-Hamiltonienne pour eux. Cette approche fournit une équation de Liouville à partir de laquelle l'Entropie peut être définie. Un résultat étonnant devient: pour les distributions de l'équilibre, la fonction de Liouville et l'Entropie du système dépendent de l'énergie. La conclusion philosophique est que une représentation dual déterministe-probabiliste des systèmes généraux est implicite dans leur nature, c'est à dire, la représentation probabiliste ne peut pas nécessairement venir d'un niveau inférieur de description.

Key words

Dynamic systems; Liouville's equation; Entropy; Energy.

Mots-clés

Systèmes dynamiques; Equation de Liouville ; Entropie ; Energie.

1. Introduction

One of the aims of General Systems Theory is opening new ways of research to understand better complexity. The general systems here considered are dynamic systems modeled by first order differential equation systems (FODES, from now onwards). The aim of this contribution is to attempt to state a thermodynamic theory for these systems. This approach could help us to understand better the nature of complexity if thermodynamic functions or variables such as temperature can be defined in the context of these systems.

Take into account that many system methodologies that have been developed ending the 20th century and starting the 21th one have contributed with systems modeled by first order differential

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[1] This article is dedicated to Lorenzo Ferrer Figueras, President of the Spanish Society of General Systems (SESGE) until his final departure; Master and friend, he always will be present in our memory.

equations. For instance, Forrester's methodology (Forrester, 1961, 1970) or Caselles's methodology (Caselles, 1992, 1993, 1994, 1995), contributes with this kind of models. In addition, the chemical reaction dynamics can be modeled with a similar manner. Thus, we present here a possible way to obtain a thermodynamics for these systems.

The unification here proposed was a central Prigogine's aim, and he had many contributions following this idea. See for instance (Prigogine, George, Henin & Rosenfeld, 1973). The dynamic systems considered in his work were physical systems, which are modeled by coupled sets of second order differential equations. My hypothesis is that a central problem to relate thermodynamics and physical dynamic systems is that thermodynamics has a first order mathematical differential structure.

A similar and present work of investigation in this field is Synergetics (Haken, 2004). This work is an attempt to unify in a unique theory, thermodynamics, information theory, dynamics and randomness, i.e., a serious and rigorous attempt to understand complexity. On the other hand, the way followed in this paper is different; it is provided through obtaining a Lagrangian-Hamiltonian formalism for FODES.

The philosophical idea is that a dual deterministic-probabilistic picture of general systems is implicit in their nature. Thus, a probability density in the space of states can be stated. In other words, the probabilistic picture would be implicit at any level of description where a system is modeled. On the other hand, the probabilistic picture would not arise necessarily from a lower level of description.

Mathematically, once known the probability density in the space of states, the thermodynamics would happen through Gibbs' equation that relates the entropy and the probability density. The mathematical procedure to obtain the probability density is the following. Pontryagin's hamiltonian function (Pontryagin, 1986) is considered for FODES. Thus, Liouville's equation takes place for the probability density in the space of states. The mathematical structure of Liouville's equation can be reorganized in such a way that holds the conservation probability equation in the space of states. Steady states are considered for this function in order to work with equilibrium thermodynamics. In a scenario of equilibrium, Entropy can be deduced as a function of the energy of system.

2. The Lagrangian-Hamiltonian approach and Liouville's equation

Let $q_i(t)$ the abstract variables depending on the time variable t of a FODES, with $i=1,2,..n$. A system like this can be represented as:

$$\frac{dq_i(t)}{dt} = f_i(t, \boldsymbol{q}(t)) \tag{1}$$

In (1) the functions f_i have all the topological properties of smoothness normally considered. The formalism here developed starts from the Lagrangian-Hamiltonian approach provided by Pontryagin (1986). This approach considers an integral optimization of a function known as Action $A(t)$:

$$A(t) = -\int V\big(t, \boldsymbol{q}(t)\big)dt \tag{2}$$

In (2), $V\big(t, \boldsymbol{q}(t)\big)$ is called *Potential*, and it represents the function to be optimized in each instant. Due to the dynamics of the vector $\boldsymbol{q}(t)$ is given by (1), this dynamics is inserted in (2) by using the Lagrange's multipliers $\lambda_i(t)$ $i=1,2,..n$. The outcome is that a new Action must be optimized:

$$S(t) = \int\left[-V(t,\boldsymbol{q}(t)) + \sum_i \lambda_i(t)(\dot{q}_i(t) - f_i(t,\boldsymbol{q}(t)))\right]dt \tag{3}$$

In (3), $\dot{q}_i(t) = \frac{dq_i}{dt}$. Observe from (3) that the following Lagrangian function can be defined:

$$L(t,\lambda_i(t),q_i(t),\dot{q}_i(t)) = \sum_i \lambda_i(t)(\dot{q}_i(t) - f_i(t,\boldsymbol{q}(t))) - V(t,\boldsymbol{q}(t)) \tag{4}$$

In (4) the abstract variables $q_i(t)$ and $\lambda_i(t)$ have the conjugated canonical momenta $p_i(t)$ defined as (from now onwards the explicit dependence on *t* is avoided in order to simplify the writing):

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = \lambda_i \tag{5}$$

Thus, the Hamiltonian function obtained from (4) and (5) is:

$$H(t,q_i,p_i) = \sum_i \dot{q}_i p_i - L = \sum_i p_i f_i(t,\boldsymbol{q}) + V(t,\boldsymbol{q}) \tag{6}$$

The canonical equations are:

$$\frac{dq_k}{dt} = \frac{\partial H}{\partial k} = f_k(t,\boldsymbol{q}) \tag{7.1}$$

$$\frac{dp_k}{dt} = -\frac{\partial H}{\partial q_k} = -\sum_i p_i \frac{\partial f_i(t,\boldsymbol{q})}{\partial q_k} - \frac{\partial V(t,\boldsymbol{q})}{\partial q_k} \tag{7.2}$$

Note that Equations (7.1) and (7.2) can be obtained through Euler-Lagrange’s equations by using the Lagrangian function (4). Equations (7.1) and (7.2) provide the dynamics for $q_k(t)$ and for $\lambda_k(t)$. In addition, by Equation (5): $p_k = \lambda_k$.

Liouville´s equation for Liouville´s function, $\rho(t,\boldsymbol{p},\boldsymbol{q})$, which represents the density function in the space of states $(\boldsymbol{p},\boldsymbol{q})$, provides the conservation in time of this function:

$$\frac{d\rho(t,\boldsymbol{p},\boldsymbol{q})}{dt} = \frac{\partial\rho(t,\boldsymbol{p},\boldsymbol{q})}{\partial t} + \sum_k \frac{\partial\rho(t,\boldsymbol{p},\boldsymbol{q})}{\partial q_k}\frac{dq_k}{dt} + \sum_k \frac{\partial\rho(t,\boldsymbol{p},\boldsymbol{q})}{\partial p_k}\frac{dp_k}{dt} = 0 \tag{8}$$

If we take into account that in our context only self-organized systems are analyzed, and not systems organized from their environment, the potential *V* must be zero in (8). In addition, considering (7-1), (7-2) and (5) in Equation (8):

$$\frac{\partial\rho(t,\boldsymbol{\lambda},\boldsymbol{q})}{\partial t} + \sum_k \frac{\partial\rho(t,\boldsymbol{\lambda},\boldsymbol{q})}{\partial q_k} f_k(t,\boldsymbol{q}) - \sum_k \sum_i \frac{\partial\rho(t,\boldsymbol{\lambda},\boldsymbol{q})}{\partial \lambda_k}\lambda_i \frac{\partial f_i(t,\boldsymbol{q})}{\partial q_k} = 0 \tag{9}$$

3. The probability density and the Entropy

Let us to demonstrate that from Liouville’s Equation (9) the fact that the square of Liouville´s function $\rho^2(t,\boldsymbol{\lambda},\boldsymbol{q})$ is a probability density can be deduced. The first step is to use the gradient symbol in (9) (the dependences on time and variables are avoided now in order to facilitate the writing demonstration):

$$\frac{\partial\rho}{\partial t} + \boldsymbol{f}\cdot\nabla_{\mathrm{q}}\rho + \boldsymbol{F}\cdot\nabla_{\lambda}\rho = 0 \tag{10}$$

Where, in (10), $\boldsymbol{f} = (f_1, \dots, f_n)$, $\nabla_{\mathrm{q}} = (\frac{\partial}{\partial q_1}, \dots, \frac{\partial}{\partial q_n})$, $\boldsymbol{F} = (-\sum_i \lambda_i \frac{\partial f_i(t,q)}{\partial q_1}, \dots, -\sum_i \lambda_i \frac{\partial f_i(t,q)}{\partial q_n})$, $\nabla_{\lambda} = (\frac{\partial}{\partial \lambda_1}, \dots, \frac{\partial}{\partial \lambda_n})$, and the point $\cdot$ means the vector product. The term $\frac{\rho}{2}\nabla_{\mathrm{q}}\boldsymbol{f}$, where $\nabla_{\mathrm{q}}\boldsymbol{f}$ is the divergence of the vector $\boldsymbol{f}$, is added and rested in (10):

$$\frac{\partial\rho}{\partial t} + \boldsymbol{f}\cdot\nabla_{\mathrm{q}}\rho + \frac{\rho}{2}\nabla_{\mathrm{q}}\boldsymbol{f} + \boldsymbol{F}\cdot\nabla_{\lambda}\rho - \frac{\rho}{2}\nabla_{\mathrm{q}}\boldsymbol{f} = 0 \tag{11}$$

In addition, if $\nabla_{\lambda}\boldsymbol{F}$ is the divergence of the vector $\boldsymbol{F}$, we have that:

$$-\nabla_{\lambda}\boldsymbol{F} = -\sum_k \frac{\partial}{\partial\lambda_k}\left(-\sum_i \lambda_i \frac{\partial f_i(t,q)}{\partial q_k}\right) = \sum_k \sum_i \delta_{ik} \frac{\partial f_i(t,q)}{\partial q_k} = \sum_k \frac{\partial f_k(t,q)}{\partial q_k} = \nabla_{\mathrm{q}}\boldsymbol{f} \tag{12}$$

Substituting (12) in (11) for the term $-\frac{\rho}{2}\nabla_{\mathrm{q}}\boldsymbol{f}$:

$$\frac{\partial\rho}{\partial t} + \boldsymbol{f}\cdot\nabla_{\mathrm{q}}\rho + \frac{\rho}{2}\nabla_{\mathrm{q}}\boldsymbol{f} + \boldsymbol{F}\cdot\nabla_{\lambda}\rho + \frac{\rho}{2}\nabla_{\lambda}\boldsymbol{F} = 0 \tag{13}$$

Multiplying (13) per 2ρ:

$$2\rho\frac{\partial\rho}{\partial t} + 2\rho\boldsymbol{f}\cdot\nabla_{\mathrm{q}}\rho + \rho^2\nabla_{\mathrm{q}}\boldsymbol{f} + 2\rho\boldsymbol{F}\cdot\nabla_{\lambda}\rho + \rho^2\nabla_{\lambda}\boldsymbol{F} = 0 \tag{14}$$

The result obtained is:

$$\frac{\partial\rho^2}{\partial t} + \nabla_{\mathrm{q}}(\boldsymbol{f}\rho^2) + \nabla_{\lambda}(\boldsymbol{F}\rho^2) = 0 \tag{15}$$

Now, the probability current vector $\boldsymbol{J}(t, \boldsymbol{\lambda}, \boldsymbol{q})$ in the 2n dimensional space of states is defined as:

$$\boldsymbol{J}(t, \boldsymbol{\lambda}, \boldsymbol{q}) = (\boldsymbol{f}, \boldsymbol{F}) = (f_1, \dots, f_n, F_1, \dots, F_n) \tag{16}$$

And the *2n* dimensional space of states gradient ***grad*** as:

$$\boldsymbol{grad} = (\nabla_{\mathrm{q}}, \nabla_{\lambda}) = (\frac{\partial}{\partial q_1}, \dots, \frac{\partial}{\partial q_n}, \frac{\partial}{\partial \lambda_1}, \dots, \frac{\partial}{\partial \lambda_n}) \tag{17}$$

Thus, from (16) and (17), Equation (15) can be reformulated as:

$$\frac{\partial\rho^2(t,\lambda,q)}{\partial t} + \boldsymbol{grad}\left(\rho^2(t,\boldsymbol{\lambda},\boldsymbol{q})\boldsymbol{J}(t,\boldsymbol{\lambda},\boldsymbol{q})\right) = 0 \tag{18}$$

Observe that (18) is the dynamic equation that represents the conservation of probability density $\rho^2(t, \boldsymbol{\lambda}, \boldsymbol{q})$, with a probability current vector given by $\boldsymbol{J}(t, \boldsymbol{\lambda}, \boldsymbol{q})$.

Once the probability density $\rho^2(t, \boldsymbol{\lambda}, \boldsymbol{q})$ is computed by solving (18), Gibbs' Entropy *S(t)* can be evaluated as:

$$S(t) = -k_B \iint \rho^2(t, \boldsymbol{\lambda}, \boldsymbol{q})\ ln(\rho^2(t, \boldsymbol{\lambda}, \boldsymbol{q}))\ d^n\boldsymbol{q}\ d^n\boldsymbol{\lambda} \tag{19}$$

In (19), k_B is Boltzman's constant. However, working with density Gibbs' Entropy $\Omega(t, \lambda, q)$ is more convenient:

$$\Omega(t, \lambda, q) = \frac{dS(t)}{d^n q\ d^n \lambda} = -k_B\ \rho^2(t, \boldsymbol{\lambda}, \boldsymbol{q})\ ln(\rho^2(t, \boldsymbol{\lambda}, \boldsymbol{q})) \tag{20}$$

4. The Entropy and the Temperature of equilibrium distributions

Following Statistical Physics, the first cases to investigate are those that provide the equilibrium distributions of (18). However, (18) is equivalent to (9), such as it has been demonstrated in the last section. Moreover, working mathematically with (9) is simpler. Actually, the equilibrium Liouville's equation is obtained from (9). The function obtained from this equation elevated to the square provides the equilibrium distribution.

First of all, observe that the search of equilibrium distributions obligates to consider autonomous systems, i.e., $f_k(t, \boldsymbol{q}) = f_k(\boldsymbol{q})$ in (1). For autonomous systems the Hamiltonian function is conserved in time. Let *E* be the constant and let it be the energy of the system. Thus, from (6) and taking into account (5) and the self-organized case, *V=0*:

$$\sum_i \lambda_i f_i(\boldsymbol{q}) = \mathrm{E} \tag{21}$$

In order to find the equilibrium Liouville's function, Statistical Physics states that $\frac{\partial \rho}{\partial t} = 0$ must be held. Let $\omega(\boldsymbol{\lambda}, \boldsymbol{q})$ be this function, thus, from (9):

$$\sum_k \frac{\partial \omega(\lambda, q)}{\partial q_k} f_k(\boldsymbol{q}) - \sum_k \sum_i \frac{\partial \omega(\lambda, q)}{\partial \lambda_k} \lambda_i \frac{\partial f_i(q)}{\partial q_k} = 0 \tag{22}$$

The solution of (22) together the condition (21) provides the equilibrium Liouville's function $\omega(\boldsymbol{\lambda}, \boldsymbol{q})$. Once normalized to the unit in the space of states $(\boldsymbol{\lambda}, \boldsymbol{q})$, equilibrium Gibbs' Entropy $\Omega(\lambda, q)$ can be evaluated from (20):

$$\Omega(\lambda, q) = -k_B\ \omega^2(\boldsymbol{\lambda}, \boldsymbol{q})\ ln(\omega^2(\boldsymbol{\lambda}, \boldsymbol{q})) \tag{23}$$

From (23), thermodynamic magnitudes such as temperature $T(\boldsymbol{\lambda}, \boldsymbol{q})$ in equilibrium can be evaluated. It is known in Statistical Physics that $T(\boldsymbol{\lambda}, \boldsymbol{q})$ can be computed as:

$$\frac{1}{T(\lambda, q)} = \frac{d\Omega(\lambda, q)}{dE} \tag{24}$$

5. Dependence on energy of equilibrium Liouville's equation

The case *n*=1 for equilibrium Liouville's function provides from (21) and (22):

$$\mathrm{E}(\lambda, q) = \lambda f(q) \tag{25}$$

$$\frac{\partial \omega(\lambda, q)}{\partial q} f(q) - \lambda f'(q) \frac{\partial \omega(\lambda, q)}{\partial \lambda} = 0 \tag{26}$$

Equation (26) is a first order linear partial differential equation. Its characteristic equations are:

$$\frac{dq}{f(q)} = \frac{d\lambda}{-\lambda f\prime(q)} = \frac{d\omega}{0} \tag{27}$$

In Equations (27) two of them can be chosen as independent:

$$\left.\begin{array}{r} \frac{d\omega}{d\lambda} = 0 \\ \frac{dq}{d\lambda} = \frac{f(q)}{-\lambda f\prime(q)} \end{array}\right\} \tag{28}$$

The solution of the system (28) in terms of two integration constants, k_1 and k_2 is:

$$\left.\begin{array}{r} \omega = k_1 \\ \lambda f(q) = k_2 \end{array}\right\} \tag{29}$$

And the solution of (26) in terms of the two integration constants is $k_1 = G(k_2)$, where *G* is an arbitrary function. Substituting the outcomes of these two constants, and seeing that k_2 is, from (25), the energy:

$$\omega(\lambda, q) = G(E(\lambda, q)) \tag{30}$$

The conclusion from (30) is that equilibrium Liouville's function is an arbitrary function of the energy of the system, being this energy computed by (25). This result suggests that the generalization for an arbitrary *n*, i.e., for Equation (22), is the same of (30), after substituting (25) for the n-dimensional energy given by (21):

$$\omega(\boldsymbol{\lambda}, \boldsymbol{q}) = G(E(\boldsymbol{\lambda}, \boldsymbol{q})) \tag{31}$$

In (31), the Energy $E(\boldsymbol{\lambda}, \boldsymbol{q})$ is given by (21). The result (31) can be proved by the direct substitution of (21) in (22).

However, a last problem must be solved. The Energy (21) is zero for the critical points of the dynamics. But due to $\omega^2(\boldsymbol{\lambda}, \boldsymbol{q})$ must be normalized, the integration on the space of states provides a discontinuity for each critical point. How to solve this mathematical problem and how to articulate the applications will be the subjects of other works.

6. Conclusions

Three results must be emphasized as conclusions of this paper. The first one is that a probabilistic picture can be deduced from the Lagrangian-Hamiltonian approach for FODES. There exists, thus, a dual deterministic-probabilistic picture for these systems. The importance of this duality is that both parts are related. In addition, the probabilistic part is not a consequence of the noise produced by the environment, but it is implicit at its mathematical nature.

The second result is that the probabilistic picture, given by the solution of Louville's equation, provides the way to compute Gibb's Entropy. Then, the Entropy can be computed from the differential formulation of the system. It permits to obtain other thermodynamic functions such as temperature. That is, the approach presented permits to state a general thermodynamics of systems.

The third result is that, for autonomous systems, both the equilibrium distribution given by Liouville’s equation and the consequent Entropy depend on the system energy. This amazing outcome is challenger in order to continue with this field of investigation.

The conclusions about future applications are not here articulated because there are many problems for the author to be elucidated. This work is only a first step to research in the field of complexity focused from the Lagrangian-Hamiltonian formalism here stated. However, the fact that a probabilistic picture can be deduced from the differential structure of a dynamic system is actually important to be considered. Moreover, this way should be investigated more due to from this probabilistic picture a general definition of Entropy can be provided and further features about complexity can be provided in a future.

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