

Poisson structure for hyperbolic heat conduction

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ABSTRACT. We use the method of extending the space of macroscopic variables (Gambár and Márkus, 1994) to construct a Hamilton-Lagrange scheme for hyperbolic transport. Specifically, we propose a Lagrangian density to obtain the telegraphist type equations as the Euler-Lagrange equation of a Hamilton variational principle. Two evolution equations for the components of a conjugated variables space are obtained from the modified Hamilton principle. These equations are particular cases of a more general time evolution equations which contains a Poisson bracket with the Hamiltonian density as the movement generator. The bracket satisfies the Jacobi's identity giving us a Poisson structure for the problem. We discuss some aspects of the time evolution of fluctuations of the temperature in a rigid heat conductor solid.

RESUMEN. En este trabajo se extiende el espacio de variables termodinámicas (Gambár y Márkus, 1994) para construir un esquema hamiltoniano para el transporte hiperbólico de calor. Específicamente se usa una densidad lagrangiana para obtener la ecuación del telegrafista como la ecuación de Euler-Lagrange de un principio variacional tipo Hamilton. Se obtienen dos ecuaciones de evolución para las variables conjugadas del espacio termodinámico desde este principio hamiltoniano. Estas ecuaciones son un caso particular de las ecuaciones de evolución definidas por los paréntesis de Poisson con el hamiltoniano como generador de la evolución temporal. El paréntesis satisface la identidad de Jacobi. Se discuten algunos aspectos de la evolución temporal de las fluctuaciones de la temperatura en un conductor rígido de calor.

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1. INTRODUCTION

The search of variational formulations of thermodynamics has a long history and has been an active field since its beginnings. In the classical theory for equilibrium systems the properties of entropy may be stated in the form of a variational principle for adiabatic processes [1, 2]. Although limited at first to non-dissipative cases, Hamilton's principle has been one of the most successful applications in non-equilibrium systems [3, 4]. As it is known, dissipative effects in real systems do not permit the direct use of Hamilton's principle but they force us to introduce the so called principles of the restricted type [5-10].

Nevertheless, it has been a subject of discussion, if classical variational principles may be formulated in some way for real systems. One may recall that, if the operators appearing in the macroscopic time evolution equations of the system are not self-adjoint, then a classical variational principle does not exist for them [11]. Since the operators of the equations of dissipative systems are not self-adjoint, the same conclusion follows. However, as Grmela and Lebon have shown [12], it is possible to construct a Poisson scheme for dissipative systems directly by defining a bracket that takes into account the dissipative contribution without going through a variational formulation. Grmela and Lebon wrote a general time evolution equation which implies the basic equations derived in the linear version of extended irreversible thermodynamics (EIT) and the dynamic equations are generated by a functional that has the meaning of a free energy.

In a different perspective, some progress has been recently reported about the problem of the existence of a classical variational principle for real systems. Sieniutycz and Berry [13] construct a Lagrangian for the thermal field as the sum of a kinetic potential and the scalar product of the constrain expressions of the process and their Lagrange multipliers. The kinetic potential depends on the field variables of an enlarged space containing not only the classical variables but also the velocity of the entropy transfer. Among the constraint expressions they include the product of entropy source and a Lagrange multiplier which is called the thermal phase. Under these conditions they develop a variational principle for real fluids containing the first and second law of thermodynamics. This leads them to a modified class of balance equations of the conserved densities.

On a different approach, Gambár and Márkus [14–18] have developed a Hamilton-Lagrange variational formalism for the parabolic equations of intensive field quantities Γ_i in the linear regime of non-equilibrium thermodynamics (LIT). The basic idea lies in the general method of construction of variational principles through the introduction of potential functions associated to the intensive field quantities Γ_k [19]. Since this point of view shares some of the motivations underlying this work, we sketch the Márkus and Gambár's method. Their starting point are equations of the diffusive type which take the form

$$\rho S_{ik}^{-1} \Gamma_{k,t} + L_{ik} \Delta \Gamma_k = \sigma_i, \quad (1)$$

where S_{ik} and L_{ik} are constant coefficients, ρ is the mass density and σ_i are given source functions, Δ is the Laplace operator and $\Gamma_{k,t} \equiv \frac{\partial \Gamma_k}{\partial t}$. By introducing new field quantities ϕ_i , whose definition depends on the intensive variable Γ_i , they are able to obtain the transport equations (1) as the Euler-Lagrange conditions of a classical variational principle. The introduction of these potential functions also allows one to find a Hamilton formalism for the equations of the ϕ 's and the corresponding equations for the associated momenta. Márkus and Gambár use their formalism to derive other interesting results of linear irreversible thermodynamics (LIT) as the balance equation for entropy and the Onsager's reciprocal relations. The latter ones are obtained from the invariance properties of the entropy production.

It is the aim of this work to use the method of introducing the new potential functions to construct a variational formulation for the hyperbolic transport equations of intensive field quantities. This kind of equations has had broad application in several fields of

theoretical physics and biology and its derivation from first principles has been studied by Olivares-Robles and García-Colín [20], Masoliver and Weiss [21] and Sancho [22].

In what follows, we will particularly show how to obtain a classical variational formulation for the telegraphist equation by defining a potential function and an action integral whose arguments are this potential and its derivatives up to second order. The Euler-Lagrange equation of this action integral will be the telegraphist equation for the field variable of interest and a corresponding equation for the potential function. Next we will transform the Lagrangian density to obtain the associated Hamiltonian description of the system by means of two equations of the Hamilton type. One equation describes the potential, the other one the associated momentum defined through a well know relation of classical mechanics. This momentum will have a direct interpretation in terms of the field variable and together with the potential function constitute a pair of conjugated field variables for the system. In the next part of the work we will discuss the associated Poisson structure of the problem. We will begin by defining a Poisson bracket which will permit us to write a general time evolution equation for any function of the potential and the conjugated momentum. This equation will particularly contain the Hamilton equations for the conjugated variables. Finally, we will prove Jacobi's identity to close the Poisson structure for the system. We apply the scheme to the case of a rigid heat conductor where we discuss some aspects about the time evolution of fluctuations in the temperature field.

2. THE INTRODUCTION OF THE FIELD POTENTIALS AND THE VARIATIONAL PROBLEM

In this part we see how a classical variational scheme for the telegraphist equation may be constructed by the introduction of a new field variable. The description of transport phenomena based on the telegraphist equation requires, in principle, one dynamic field variable ϑ such that

$$\vartheta_{,tt} + \frac{1}{\tau}\vartheta_{,t} = c^2\Delta\vartheta. \quad (2)$$

We enlarge the initial space by defining a potential function ϕ (the only requirement on this function is that it must be a four times differentiable function) associated to ϑ as follows:

$$\vartheta = -\frac{1}{\tau}\phi_{,t} + \phi_{,tt} - c^2\Delta\phi. \quad (3)$$

It is then necessary to find a Lagrangian density function from which Eq. (2) may be obtained by the variation of the potential function ϕ . Let a Lagrangian density function L be depending on

$$L = L(\phi, \phi_{,t}, \phi_{,tt}, \phi_{,xx}, \phi_{,yy}, \phi_{,zz}), \quad (4)$$

which we take as

$$L = \frac{1}{2} \left[-\frac{1}{\tau}\phi_{,t} + \phi_{,tt} - c^2\Delta\phi \right]^2, \quad (5)$$

and let us consider the classical variational problem

$$\delta \iiint L dV dt = 0, \quad (6)$$

with L given in Eq. (5)

As it is known, the Euler-Lagrange equation of Eq. (6) is

$$\frac{\partial L}{\partial \phi} - \frac{\partial}{\partial t} \frac{\partial L}{\partial \phi_t} + \frac{\partial^2}{\partial t^2} \frac{\partial L}{\partial \phi_{tt}} + \frac{\partial^2}{\partial x^2} \frac{\partial L}{\partial \phi_{xx}} + \frac{\partial^2}{\partial y^2} \frac{\partial L}{\partial \phi_{yy}} + \frac{\partial^2}{\partial z^2} \frac{\partial L}{\partial \phi_{zz}} = 0. \quad (7)$$

Substitution of the Lagrangian density as defined in Eq. (5) into the Euler-Lagrange equation (7) gives

$$\begin{aligned} & \frac{1}{\tau} \frac{\partial}{\partial t} \left(-\frac{1}{\tau} \phi_{,t} + \phi_{,tt} - c^2 \Delta \phi \right) + \frac{\partial^2}{\partial t^2} \left(-\frac{1}{\tau} \phi_{,t} + \phi_{,tt} - c^2 \Delta \phi \right) + \\ & c^2 \frac{\partial^2}{\partial x^2} \left(-\frac{1}{\tau} \phi_{,t} + \phi_{,tt} - c^2 \Delta \phi \right) + c^2 \frac{\partial^2}{\partial y^2} \left(-\frac{1}{\tau} \phi_{,t} + \phi_{,tt} - c^2 \Delta \phi \right) + \\ & c^2 \frac{\partial^2}{\partial z^2} \left(-\frac{1}{\tau} \phi_{,t} + \phi_{,tt} - c^2 \Delta \phi \right) = 0, \end{aligned}$$

which is the telegraphist equation (2) in virtue of Eq. (3). Thus, we have a Lagrangian formulation for this equation.

Now we proceed to calculate the Hamiltonian density function H through a Legendre transform on the Lagrangian density L , Eq. (5):

$$H = \phi_{,t} \pi - L, \quad (8)$$

where the conjugated momentum π is, by definition

$$\pi = \frac{\partial L}{\partial \phi_{,t}} = -\frac{1}{\tau} \vartheta. \quad (9)$$

We note that the conjugated momentum π has a direct physical meaning in terms of the field variable ϑ and τ , the relaxation time associated to ϑ .

Introducing π in the Legendre transform, Eq. (8), we obtain

$$H = -\frac{1}{\tau} \phi_{,t} \vartheta - \frac{1}{2} \vartheta^2. \quad (10)$$

Observing that $\phi_{,t}$ is given by

$$\phi_{,t} = -\tau(\vartheta - \phi_{,tt} + c^2 \Delta \phi), \quad (11)$$

we can rewrite H as

$$H = \frac{1}{2}\vartheta^2 + (c^2\Delta\phi - \phi_{,tt})\vartheta. \quad (12)$$

Finally, in terms of the conjugated momentum π we arrive to

$$H(\pi, \square\phi) = \frac{1}{2}(\tau\pi)^2 - \tau\pi\square\phi, \quad (13)$$

where we have introduced the d'Alembert operator \square defined as

$$\square \equiv c^2\Delta - \frac{\partial^2}{\partial t^2}. \quad (14)$$

At this point we pose the problem in terms of the modified Hamilton's variational principle

$$\delta \iiint (\pi\phi_{,t} - H) dV dt = 0, \quad (15)$$

in order to arrive to the Hamiltonian equations for the conjugated variables π and ϕ , where the Hamiltonian density H is given in Eq. (13). Observing that H depends on π and $\square\phi$, Eq. (15) becomes

$$\iiint dV dt \left[\pi \delta\phi_{,t} + \phi_{,t} \delta\pi - \frac{\partial H}{\partial \pi} \delta\pi - \frac{\partial H}{\partial \square\pi} \delta\square\phi \right] = 0.$$

After some straightforward algebra we obtain that

$$\iiint dV dt \left[\left(\phi_{,t} - \frac{\partial H}{\partial \pi} \right) \delta\pi - \left(\pi_{,t} + \square \frac{\partial H}{\partial \square\pi} \right) \delta\phi \right] = 0. \quad (16)$$

Being $\delta\pi$ and $\delta\phi$ independent variations, the Hamilton equations are thus given by

$$\phi_{,t} = \frac{\partial H}{\partial \pi}, \quad (17)$$

$$\pi_{,t} = -\square \frac{\partial H}{\partial \square\pi}. \quad (18)$$

Equations (17) and (18) are the dynamic equations for ϕ and π . It may be shown that Eq. (18) gives the telegraphist equation for the momentum π or for ϑ according to Eq. (9) when the result of Eq. (13) is introduced in it. Eq. (17) gives the equation for the potential function ϕ

$$\phi_{,tt} + \frac{1}{\tau_q}\phi_{,t} - c^2\Delta\phi = \frac{1}{\tau}\vartheta, \quad (19)$$

which is precisely the definition of ϕ .

In the next section we address ourselves to formulate a convenient form for a Poisson bracket to include Eqs. (17) and (18) as particular cases of a general time evolution equation. This equation will have an important meaning since it will permit us to describe the time evolution of any dynamic density depending on the conjugated variables π and ϕ and, at the same time, it will exhibit that the Hamiltonian density H of Eq. (13) plays the relevant role of the generator of the time evolution of the system.

3. POISSON STRUCTURE FOR HYPERBOLIC TRANSPORT

Given the previous Hamiltonian formulation for the hyperbolic transport Eq. (2), it is possible to formulate the problem in a natural way in terms of a Poisson bracket. This bracket is defined for any pair of densities A and B as

$$\{A, B\} = \frac{\delta A}{\delta \phi} \frac{\Delta B}{\delta \pi} - \frac{\delta B}{\delta \phi} \frac{\delta A}{\delta \pi}, \quad (20)$$

where we have introduced the operators $\frac{\delta}{\delta \phi}$ and $\frac{\delta}{\delta \pi}$ as

$$\frac{\delta}{\delta \phi} \equiv \frac{\partial}{\partial \phi} - \nabla \cdot \frac{\partial}{\partial \nabla \phi} + \square \frac{\partial}{\partial \square \phi}, \quad (21)$$

and

$$\frac{\delta}{\delta \pi} \equiv \frac{\partial}{\partial \pi} - \nabla \cdot \frac{\partial}{\partial \nabla \pi} + \square \frac{\partial}{\partial \square \pi}. \quad (22)$$

Here we have assumed that

$$A = A(\phi, \nabla \phi, \square \phi, \pi, \nabla \pi, \square \pi), \quad (23)$$

$$B = B(\phi, \nabla \phi, \square \phi, \pi, \nabla \pi, \square \pi). \quad (24)$$

Under these conditions the dynamic Eqs. (17) and (18) may be regarded as particular cases of the general equation

$$A_{,t} = \{A, H\}, \quad (25)$$

A being any density depending on the conjugated variables ϕ and π . If, for instance, $A = \phi$ then Eq. (25) gives Eq. (17) and if $A = \pi$, Eq. (18) is obtained.

We complete the scheme by showing that the Poisson bracket satisfies Jacobi's identity, namely

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0. \quad (26)$$

All we need to see is that $\{, \}$ as defined by Eq. (20) is a linear operator

$$\{A, \lambda(B + C)\} = \lambda\{A, B\} + \lambda\{A, C\}.$$

But this is easy to prove since $\frac{\delta}{\delta\phi}$ and $\frac{\delta}{\delta\pi}$ are linear operators. If one expands each term of Eq. (26) two kinds of expressions are obtained. One is of the form

$$\frac{\delta A}{\delta\chi} \frac{\delta B}{\delta\chi} \frac{\delta^2 C}{\delta\zeta^2},$$

and the other one is

$$\frac{\delta A}{\delta\chi} \frac{\delta B}{\delta\zeta} \frac{\delta^2 C}{\delta\chi\delta\zeta},$$

where χ and ζ may be either ϕ or π . Other terms are obtained by permutations of A , B , and C in such expressions. Each one of these terms has its additive inverse in the complete expansion of the left hand side of Eq. (26) giving the desired result. Now we particularize the above results for the case of a rigid solid heat conductor.

4. HYPERBOLIC HEAT CONDUCTION

In this section we deal with the hyperbolic transport of heat in a rigid conductor solid where the heat is propagating by conduction through waves at finite speeds [23]. The theoretical importance of the problem may be appreciated in the extensive review of Joseph and Preziosi [24, 25] and it has been in the interest of many groups during the last thirty years [26–34]. Here we consider the telegraphist equation for the temperature as the model of hyperbolic heat conduction. This equation may be obtained through a general constitutive equation for the heat flux derived by means of a variational principle of the restricted type [35]. Up to second order the constitutive equation reduces to

$$\tau_q \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -K \nabla T, \quad (27)$$

considering an homogeneous heat flux. This equation is a well known result in the theory of viscoelastic fluids and solids and in relaxing gas dynamics.

By combining the balance equation

$$\rho \frac{de}{dt} = -\nabla \cdot \mathbf{q}, \quad (28)$$

with the constitutive equation, Eq. (27) we arrive to the corresponding hyperbolic transport equation for the rigid heat conductor solid

$$T_{,tt} + \frac{1}{\tau_q} T_{,t} = c^2 \Delta T, \quad (29)$$

where τ_q is the relaxation time of the heat flux and $c^2 = K/\rho C_v \tau_q$, with K the thermal conductivity and C_v the specific heat.

In the Hamiltonian context the heat conductor is then described by the conjugated field variables ϕ and π , being the momentum proportional to the temperature

$$\pi = -\frac{1}{\tau_q}T. \quad (30)$$

The dynamic behavior of ϕ and π is given by the extremum conditions of the variational principle Eq. (15) or by the general evolution equation (25) with the Hamiltonian density H defined as

$$H(\pi, \square\phi) = \frac{1}{2}(\tau_q\pi)^2 - \tau_q\pi\square\phi,$$

and A equal to ϕ and π , respectively.

Now we use the time evolution Eq. (25) to describe the dynamic behavior of the fluctuations in the temperature of the hyperbolic heat conductor. This is possible because we know the expression for the fluctuations of temperature in terms of the conjugated momentum π . The statistics of the thermal fluctuations in a rigid heat conductor was studied by Jou *et al.* [36] within the framework of EIT based on the Einstein formula for the probability of fluctuations. Here we then take the fluctuations with respect to a given stationary state T_{est} as

$$\delta T = -\tau_q(\pi - \pi_{\text{est}}). \quad (31)$$

Thus, the time evolution of the fluctuation is given by

$$\frac{\partial\delta T}{\partial t} = \{\delta T, H\}. \quad (32)$$

Solving, one obtains the telegraphist equation for δT

$$\frac{\partial^2\delta T}{\partial t^2} + \frac{1}{\tau_q}\frac{\partial\delta T}{\partial t} - c^2\Delta\delta T = 0. \quad (33)$$

This means that the temperature fluctuations inherit some of the properties of quantities being described by the telegraphist equation. On the other hand, if one makes the calculation presented in Eqs. (31–33) for LIT within the Márkus and Gambár framework, one finds that the temperature fluctuations obey the diffusive type transport equation (1), *i.e.*,

$$\frac{\partial\delta T_D}{\partial t} - D^2\Delta\delta T_D = 0, \quad (34)$$

where the subscript D , indicates that such fluctuations are described by a diffusive model. This fact introduces some differences in the dynamics of fluctuations between the two schemes. In order to discuss such differences we have plotted in Fig. 1 for the two cases the evolution of a fluctuation in the temperature of an infinite conducting bar initially

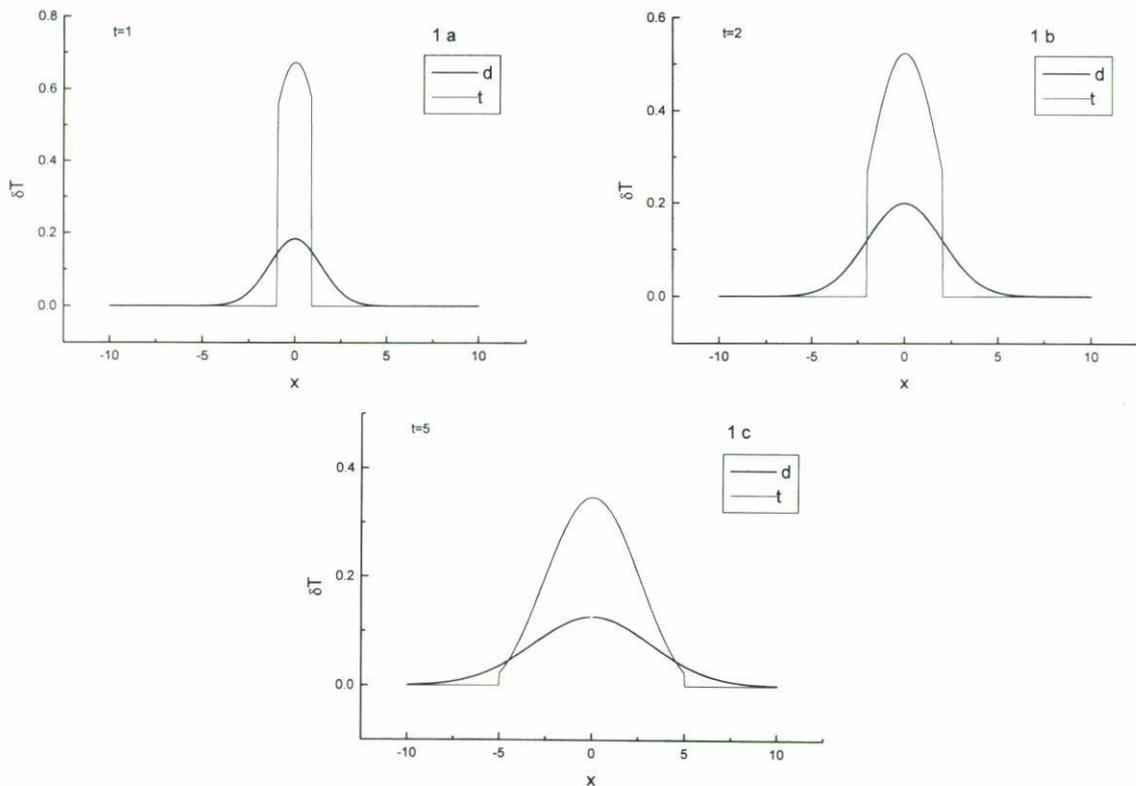


FIGURE 1. The time evolution of a Dirac's delta fluctuation of temperature initially centered at $x = 0$. The values of time are normalized and d and t refer to diffusion and telegraphist respectively.

centered at the origin of the reference coordinate system. The fluctuations have been represented by Dirac's delta function which has been taken as the initial temperature profile for the initial condition problem of the telegraphist and the diffusion equations. The plots have been obtained directly from the analytic solution for the two equations [37]. In Fig. 2 we can see the description made from two fixed point in the bar, namely, 2a at the origin and 2b at $x = 5$. Some comments are in order.

We note in all diagrams of Fig. 1 the existence of a wave front for the telegraphist solution beyond which the fluctuation in temperature of the bar vanishes. This is one of the distinctive points of the dynamical behavior of perturbations in the hyperbolic description. Signals are transmitted with a finite velocity through the medium. This may also be appreciated in the evolution of temperature at $x = 5$ in Fig. 2b where the temperature rises in $t = 5$ and then increases continuously. Before $t = 5$ the perturbation has not arrived to the point $x = 5$ of the bar. In contrast, the parabolic solution extends beyond this point of the bar. The perturbations are transmitted with a velocity much greater than the velocity in the hyperbolic case. In Fig. 2b we see that the corresponding temperature in the position $x = 5$ is not zero all the time. Mention must be made that the instantaneous jump in the temperature fluctuation in the hyperbolic case is due to

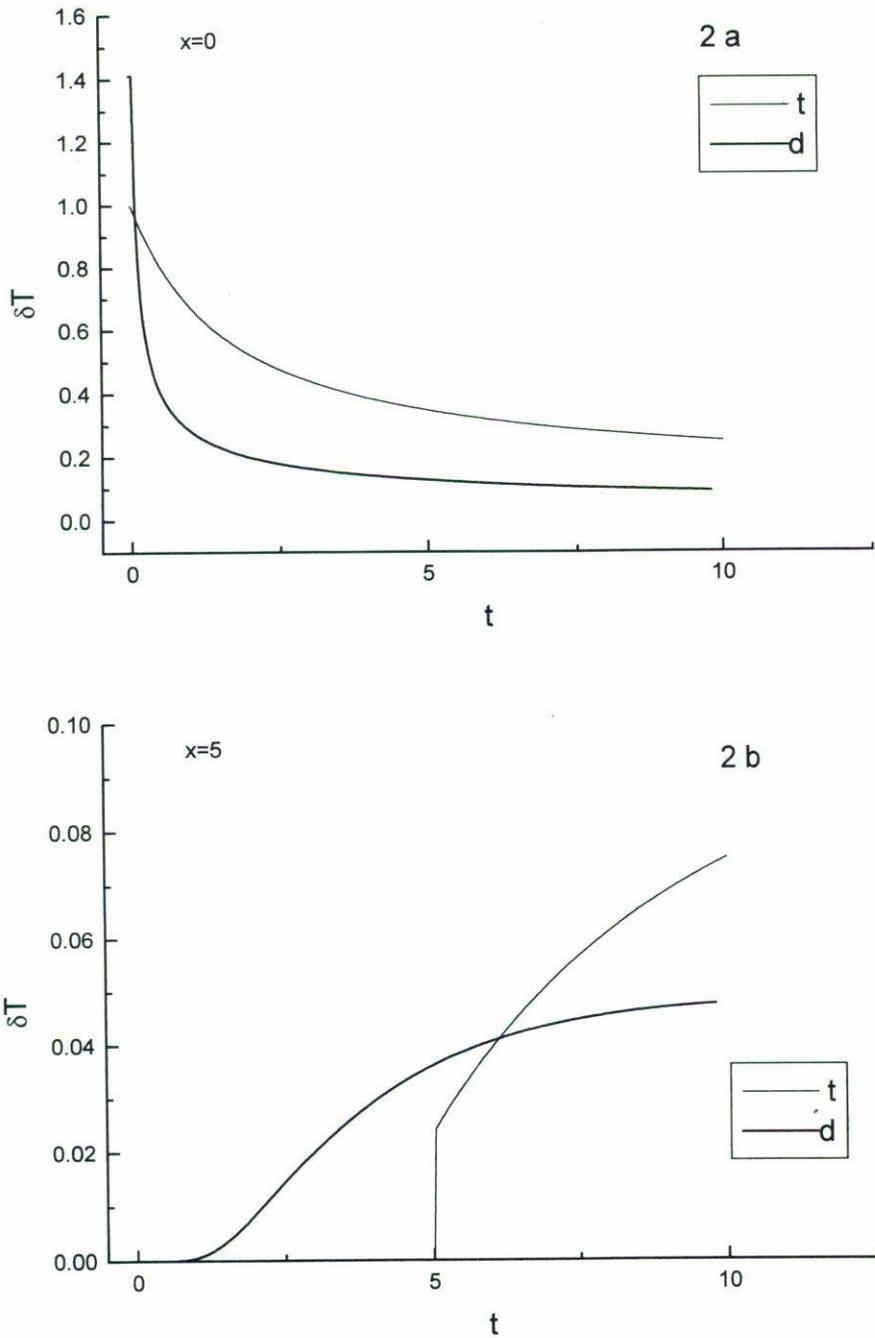


FIGURE 2. It is shown the change in time of the temperature at two fixed points $x = 0$ and $x = 5$. Time is normalized and d and t have the same meaning as in Fig. 1

the nature of the delta function taken as the initial condition to find the solution of the problem.

We now close this discussion with some final remarks.

5. CONCLUDING REMARKS

In this work we find a classical variational principle for the hyperbolic type transport equations for intensive field variables. For simplicity, we restrict ourselves to systems described by only one field quantity particularizing to the case of a rigid heat conductor. To begin with, we enlarge the space of one variable by defining a potential function which together with a defined momentum forms a pair of conjugated variables in the classical sense. A Hamilton-Lagrange formalism is obtained through a variational principle based with a conveniently defined Lagrangian density. Then we construct a bracket whose main property is to satisfy Jacobi's identity getting a Poisson structure for the problem. We have written a general time evolution equation for any density which contains as particular cases the Hamilton equations of the field. Any dynamical property of the system depending on the conjugated variables may be then described through the general time evolution equation in terms of the Poisson bracket and the Hamiltonian density as the generator of the movement in time. As an example we apply the formalism to a rigid heat conductor solid. We find that the temperature of the solid plays the role of the conjugated momentum in the Hamiltonian scheme. Finally, by writing the dynamic fluctuations of the temperature as a function of the conjugated momentum we also find that they satisfy the telegraphist equation and discuss some differences with respect to the parabolic case.

The purpose to obtain a Hamiltonian structure for nonequilibrium processes was also pursued by Sieniutycz and Berry. Their formalism also involves the idea of the enlargement of the space of independent variables of the system. However, this leads them to suggest a modification for the balance equations of the system which is not the case of the method of the potential functions used here.

The results obtained in this work deserve one additional comment. The main goal is the development of a classical variational scheme for systems whose dynamic behavior is described by a telegraphist type equation. The way we construct the variational principle maintains the steps of those used by Gambár and Márkus based on the definition of a potential function associated with each intensive quantity of the system. Nevertheless, our physical problem is different. We tackle problems which, from a thermodynamical point of view, include inertial effects. This may be seen in the case of heat transfer where we assume the Maxwell-Cattaneo-Vernotte equation for the heat flux instead of Fourier's law, in order to obtain the corresponding transport equation.

We would like to remark the fact that the fluctuations of the transported quantity obey the same telegraphist equation. This may appear obvious, but from this macroscopic perspective the Onsager's hypothesis on fluctuation regression seems to be a consequence of the relation between the conjugated momentum and the temperature Eq. (30).

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