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1990 J. Phys. A: Math. Gen. 23 3341

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Hamiltonian extended thermodynamics

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Received 3 August 1989, in final form 11 April 1990

Abstract. It is shown that the time evolution equations governing the behaviour of the thermodynamic fluxes in extended irreversible thermodynamics possess a generalised Hamiltonian structure.

1. Introduction

Extended irreversible thermodynamics has fuelled much interest during the two last decades (e.g. Casas *et al* 1984, Jou *et al* 1988). Extended irreversible thermodynamics was conceived out of the necessity to extend classical irreversible thermodynamics (Onsager 1931, Prigogine 1961, De Groot and Mazur 1962) whose domain of application is limited to steady linear constitutive equations. The second motivation of extended irreversible thermodynamics was to avoid the unpleasant property of propagation of thermal, concentration and velocity disturbances with an infinite velocity. This characteristic is inherent to the Fourier, Fick and Navier-Stokes equations as these lead to parabolic equations of balance.

Extended irreversible thermodynamics is particularly well suited for describing high frequency and small wavelength phenomena such as ultrasonic propagation in gases and metals and light and neutron scattering (Lebon and Cloot 1989, Valesco and Garcia-Colin 1983). The formalism is also useful for describing systems with large relaxation times like dielectrics (Castillo and Garcia-Colin 1986), viscoelastic and non-Newtonian fluids (Lebon and Cloot 1988, Lebon *et al* 1990, Perez-Garcia *et al* 1989). Extended irreversible thermodynamics also helped to settle the domain of validity in the classical theory of irreversible processes by defining in a precise manner the limits of application of the local equilibrium hypothesis and the Onsager-Casimir reciprocal relations.

The basic assumption in extended irreversible thermodynamics is to enlarge the space of the basic variables by completing the classical set formed by the mass, momentum and energy by means of extra variables taking the form of thermodynamic fluxes such as the mass flux, the heat flux and the flux of momentum. The second hypothesis is to assume that these extra variables satisfy non-steady (generally non-linear) evolution equations. Thirdly the existence of a non-equilibrium entropy with a non-negative production is postulated. The foundations for the above three hypotheses of extended irreversible thermodynamics are deeply rooted in the basic laws of kinetic theory, statistical mechanics and information theory (Jou *et al* 1988).

The purpose of this paper is to use still another type of argument to provide a foundation for the second and third hypotheses. The argument is based on the observation that classical irreversible thermodynamics, as well as other well established formalisms, like Boltzmann's kinetic theory or Maxwell's electrodynamic equations, possess the so-called generalised Hamiltonian structure (Clebsch 1985, Iwinski *et al* 1976, Morrison 1980, 1983, Dzyaloshinskii *et al* 1980, Grmela 1984, 1986, 1988, Kaufman 1984). The properties of the solutions of equations with a Hamiltonian structure have been interpreted by Grmela (1986, 1988) as an expression of the compatibility of the time evolution equations with equilibrium thermodynamics. There are other reasons that militate in favour of a Hamiltonian description. It is very attractive to formulate the behaviour of a whole class of phenomena in Hamiltonian form because of its conciseness and its physical contents. Indeed the whole set of balance equations is now replaced by one single relation and furthermore, the generating functional of each particular problem may generally be identified with a well-defined physical quantity like the energy, the entropy, the free Gibbs energy, etc. (Grmela 1989). Moreover, there exist many results and methods of solutions typically developed for general Hamiltonian systems (e.g. Arnold 1965, Holm *et al* 1985) which can be of direct use to analyse the solutions of the basic equations of extended irreversible thermodynamics.

It is shown in this paper that the Hamiltonian structure is preserved when the state of the basic variables is enlarged in the way advocated in extended irreversible thermodynamics. It is demonstrated in section 3 that the proposed Hamiltonian structure leads to the time evolution equations that are derived in Jou *et al* (1988). The advantages gained by using a generalised Hamiltonian formalism in extended irreversible thermodynamics are discussed in the concluding section 4. For completeness, the generalised Hamiltonian structure of classical irreversible thermodynamics will be recalled in section 2.

2. Generalised Hamiltonian structure of classical irreversible thermodynamics

We briefly recall here the generalised Hamiltonian structure of classical irreversible thermodynamics and also introduce the terminology and notation used in this paper. The state variables in classical irreversible thermodynamics are the five hydrodynamic fields: mass density $\rho(\mathbf{r}, t)$, energy $e(\mathbf{r}, t)$, and momentum $\mathbf{u}(\mathbf{r}, t)$.

We first consider the non-dissipative part of the balance laws and demonstrate their Hamiltonian structure. We say that the evolution of a variable is non-dissipative when the corresponding quantity is conserved (no production term in the balance law).

It is assumed that there exists an entropy function

$$S(t) = \int d\mathbf{r} s(\mathbf{r}, t) \quad (1)$$

such that the entropy density $s(\mathbf{r}, t)$ is a convex function of the variables ρ , e , \mathbf{u} and that for an isolated system

$$\frac{dS}{dt} = 0. \quad (2)$$

It is also supposed that there is a one-to-one transformation between the variables (ρ, e, \mathbf{u}) and (ρ, s, \mathbf{u}) for all \mathbf{r} and t . According to the classical terminology (Callen

1985), when s is the dependent and (ρ, e, \mathbf{u}) the independent variables, we shall refer to the analysis as being the entropy representation. If the energy is the dependent and (ρ, s, \mathbf{u}) the independent variables, we shall talk about energy representation.

Let A denote a sufficiently regular functional of the fields ρ, s, \mathbf{u} . Clearly, if we know the time evolution equations for ρ, s, \mathbf{u} , we also know the time evolution of A , namely

$$\frac{dA}{dt} = \frac{1}{V} \int d\mathbf{r} \left(\frac{\delta A}{\delta \rho} \partial_t \rho + \frac{\delta A}{\delta s} \partial_t s + \frac{\delta A}{\delta \mathbf{u}} \cdot \partial_t \mathbf{u} \right) \quad (3)$$

where ∂_t stands for the partial time derivative and V for the volume, supposed to be fixed, confining the system under consideration, δ is the Volterra functional differentiation. It is known that $\delta A / \delta \rho(\mathbf{r}, t)$ reduces to the usual partial derivative if the function $\rho(\mathbf{r}, t)$ is replaced by a finite dimensional vector. We note that if in particular

$$A(t) = \int d\mathbf{r} a[\rho(\mathbf{r}, t), s(\mathbf{r}, t), \mathbf{u}(\mathbf{r}, t)]$$

where a is a local sufficient regular function of ρ, s, \mathbf{u} (which means that a evaluated at \mathbf{r} depends only on the fields ρ, s, \mathbf{u} at \mathbf{r} and not at other different position vectors), then the Volterra derivatives reduce to the usual partial derivatives:

$$\frac{1}{V} \frac{\delta A}{\delta \rho(\mathbf{r}, t)} = a_\rho \quad \frac{1}{V} \frac{\delta A}{\delta s(\mathbf{r}, t)} = a_s \quad \frac{1}{V} \frac{\delta A}{\delta \mathbf{u}(\mathbf{r}, t)} = a_u$$

$a_\rho (= \partial a / \partial \rho(\mathbf{r}, t))$ etc denote the partial derivation of a with respect to ρ , etc.

Of course, if we know the time evolution equation for A and require it to hold for all sufficient regular functional A , then we can derive the time evolution equations for the fields ρ, s, \mathbf{u} . If in addition the time evolution for A can be cast into the form

$$\frac{dA}{dt} = \frac{1}{V} \{A, G\} \quad (4)$$

where $\{A, G\}$ is called a Poisson bracket and G a generating functional, then the time evolution equations for ρ, s, \mathbf{u} are said to possess the Hamiltonian structure. We recall that $\{A, G\}$ is a Poisson bracket if the following three properties are satisfied:

(i) $\{A, G\}$ is a linear function of the Volterra functional derivatives of A and G with respect to the fields ρ, s, \mathbf{u} respectively;

(ii) $\{A, G\} = -\{G, A\}$ (antisymmetry);

(iii) $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$ (Jacobi identity).

Let us select as Poisson bracket

$$\begin{aligned} \{A, G\} = & \frac{1}{V} \int d\mathbf{r} \rho \left[\left(\frac{\delta A}{\delta \rho} \right)_{,k} \frac{\delta G}{\delta u_k} - \left(\frac{\delta G}{\delta \rho} \right)_{,k} \frac{\delta A}{\delta u_k} \right] \\ & + \frac{1}{V} \int d\mathbf{r} u_i \left[\left(\frac{\delta A}{\delta u_i} \right)_{,k} \frac{\delta G}{\delta u_k} - \left(\frac{\delta G}{\delta u_i} \right)_{,k} \frac{\delta A}{\delta u_k} \right] \\ & + \frac{1}{V} \int d\mathbf{r} s \left[\left(\frac{\delta A}{\delta s} \right)_{,k} \frac{\delta G}{\delta u_k} - \left(\frac{\delta G}{\delta s} \right)_{,k} \frac{\delta A}{\delta u_k} \right] \end{aligned} \quad (5)$$

and identify the generating functional G with the total energy

$$E = \int d\mathbf{r} e(\mathbf{r}, t).$$

From now on, Cartesian coordinates and the summation convention on repeated indices are used, a comma stands for the partial derivation with respect to the spatial coordinates. We now show that equation (4) is identical to the non-dissipative part of the balance laws of classical irreversible thermodynamics together with local equilibrium relations among the fields ρ, e, s, \mathbf{u} and p (p is the local pressure). Performing integration by parts and introducing boundary conditions that guarantee that all the integrals over the surface bounding the system are zero, we can rewrite equation (4) as

$$\frac{dA}{dt} = -\frac{1}{V} \int d\mathbf{r} \left\{ \frac{\delta A}{\delta \rho} (\rho e_{u_k})_{,k} + \frac{\delta A}{\delta s} (s e_{u_k})_{,k} + \frac{\delta A}{\delta u_k} [(u_k e_{u_j})_{,j} + \rho (e_{\rho})_{,k} + u_j (e_{u_j})_{,k} + s (e_{\nu})_{,k}] \right\}.$$

Since it is demanded that equation (3) holds for any functional A , one has

$$\begin{aligned} \partial_t \rho &= -(\rho e_{u_k})_{,k} & \partial_t s &= -(s e_{u_k})_{,k} \\ \partial_t u_k &= -(u_k e_{u_j})_{,j} - \rho (e_{\rho})_{,k} - u_j (e_{u_j})_{,k} - s (e_{\nu})_{,k}. \end{aligned} \tag{6}$$

In order that expressions (6) represent the non-dissipative parts of the balance laws of classical irreversible thermodynamics one has to make the following identifications:

$$e_{u_k} = \frac{1}{\rho} u_k = v_k \tag{7}$$

where v_k is the velocity field, and

$$p_{,k} = \rho (e_{\rho})_{,k} + u_j (e_{u_j})_{,k} + s (e_{\nu})_{,k}. \tag{8}$$

Equation (8) together with

$$e_{,k} = e_{\rho} \rho_{,k} + e_{u_j} (u_j)_{,k} + e_{\nu} s_{,k} \tag{9}$$

implies

$$p = -e + s e_{\nu} + \rho e_{\rho} + u_k e_{u_k} \tag{10}$$

which is nothing but the Euler local equilibrium relation.

Now we turn our attention to the dissipative part of the evolution equations. For the sake of simplicity, we shall from now on limit the analysis to an incompressible fluid at rest. It is then an easy task to see that the equations of classical irreversible thermodynamics are recovered at the condition to replace equation (4) by

$$\frac{dA}{dt} = \frac{1}{V} \{A, G\} + \frac{1}{V} [A, G] \tag{11}$$

G stands for the total free energy

$$G = \int d\mathbf{r} (e - T_0 s) \tag{12}$$

with T_0 a constant temperature while $[A, G]$ is given by

$$[A, G] = -\frac{1}{V} \int d\mathbf{r} (A_e)_{,k} \frac{1}{G_e} \frac{\delta \Phi}{\delta (G_e)_{,k}} \tag{13}$$

where Φ is the so-called dissipative potential introduced by Moreau (1970) and Edelen (1972). The dissipative potential is required to obey the following properties:

- (i) $\Phi(0) = 0$;
- (ii) Φ reaches its minimum at zero;
- (iii) $-\Phi$ is convex in the neighbourhood of zero.

These properties are met if

$$\frac{dS}{dt} > 0. \quad (14)$$

The form of the bracket $[A, G]$ that includes the viscosity may be found in Grmela's paper (1989) to which the reader is referred for more details.

3. Generalised Hamiltonian structure of extended irreversible thermodynamics

We proceed now to the identification of the Hamiltonian structure of the governing equations of extended irreversible thermodynamics. Following Jou *et al* (1988), we select as state variables the energy field $e(\mathbf{r}, t)$, the heat flux field $\mathbf{q}(\mathbf{r}, t)$ and the viscous pressure tensor field $\mathbf{P}(\mathbf{r}, t)$. The tensor \mathbf{P} is supposed to be symmetric. For the sake of simplicity, we do not split the tensor \mathbf{P} into a diagonal and a traceless part.

The problem that we intend to solve is the following. We search for a generating functional G , a Poisson bracket $\{, \}$, and a dissipation bracket $[,]$, all defined in the state space composed by the fields $e(\mathbf{r}, t)$, $\mathbf{q}(\mathbf{r}, t)$, $\mathbf{P}(\mathbf{r}, t)$ such that

- (i) the generating functional has the physical meaning of a free energy;
- (ii) equation (11), linearised about an equilibrium state, is equivalent to the governing time-evolution equations of extended irreversible thermodynamics as given for instance in Jou *et al* (1988).

At this point, it is worth stressing that the problem has not necessarily a unique solution. This is due to the non-uniqueness of the Poisson $\{, \}$ and dissipative $[,]$ brackets. To make the choice unique, we would have to introduce supplementary restrictions; for instance, for the dissipative function defined by equation (13), one should add other requirements which complement the three properties of the dissipative function listed after equation (13). Moreover, non-uniqueness is in no way related to complete integrability. To each Hamiltonian structure correspond different evolution equations. These equations will only coincide when the analysis is restricted to equilibrium and close to equilibrium states (Grmela 1984, 1986).

The way to determine the appropriate Poisson bracket is to follow three different routes. Firstly, we can try to present the state space as dual of the semidirect product of a Lie algebra and a direct sum of vector spaces. For the state space considered in section 2, the Lie algebra is the Lie algebra of vector fields on \mathbb{R}^3 and the vector spaces are the modules of differential forms on which the vector fields act naturally by Lie derivatives: the Poisson bracket arises then naturally (Holm *et al* 1985). In the case of extended thermodynamics we do not see any physical ground to associate the corresponding state space with a Lie algebra structure (notice that the velocity field that is associated with the Lie algebra of vector fields on \mathbb{R}^3 is missing in our state space). Therefore we shall not follow this route here. The second route starts by representing the states variables $e(\mathbf{r}, t)$, $\mathbf{q}(\mathbf{r}, t)$, $\mathbf{P}(\mathbf{r}, t)$ in terms of moments of a one-particle distribution function. Next we use the Poisson bracket associated with the Hamiltonian structure of the one-particle distribution kinetic equations (Morisson

1983, Grmela 1984, 1986). By restricting the functionals A, B appearing in the Poisson bracket to depend only on the one-particle distribution functions throughout their dependence on the moments $e(r, t), q(r, t), P(r, t)$, we obtain a bracket involving these moments. The bracket will, however, also contain other moments. It is therefore necessary to look for a closure relation expressing these other moments in terms of the basic moments $e(r, t), q(r, t), P(r, t)$. The Jacobi identity may be then regarded as an equation with the closure considered as an unknown function. Unfortunately, the explicit formulation of such an equation requires a tremendous amount of calculation and therefore in the present paper, we have preferred to follow a third route. The latter is based on a trial and error technique. We suggest the form of a bracket, check explicitly that it is a Poisson bracket and verify also that equations of the form $dA/dt = (1/V)\{A, G\}$ represent the governing equations of extended irreversible thermodynamics.

3.1. The non-dissipative time evolution

In the absence of dissipation, the total entropy is conserved and one has

$$\frac{d}{dt} \int dr s(r, t) = 0 \tag{15}$$

where $s(r, t)$ is a function sufficiently regular of e, q , and P . Without any difficulty, we can allow the function s to depend in addition on the gradients of s, q and P ; this would be appropriate for the description of non-local effects. The requirement (15) of non-dissipation implies that, in the limit of a local theory,

$$\partial_i s = -J_{k,k}^s \tag{16}$$

where J_k^s is the entropy flux vector which remains unspecified at this stage of the analysis. Let A denote a sufficiently regular functional of the state variables. In the energy representation, we have

$$\frac{dA}{dt} = \frac{1}{V} \int dr \left[\frac{\delta A}{\delta s} \partial_i s + \frac{\delta A}{\delta q_k} \partial_i q_k + \frac{\delta A}{\delta P_{kl}} \partial_i P_{kl} \right]. \tag{17}$$

As stated earlier, we say that the equations governing the time evolution of s, q and P exhibit a Hamiltonian structure with the quantity G serving as generating functional it for all A ,

$$\frac{dA}{dt} = \frac{1}{V} \{A, G\}. \tag{18}$$

We shall show that by choosing as generating function the energy E and by defining the Poisson bracket by

$$\begin{aligned} \{A, G\} = & \frac{1}{V} \int dr \mu_1 \left[\left(\frac{\delta A}{\delta s} \right)_{,k} \frac{\delta G}{\delta q_k} - \left(\frac{\delta G}{\delta s} \right)_{,k} \frac{\delta A}{\delta q_k} \right] \\ & + \frac{1}{V} \int dr \mu_2 \left[\left(\frac{\delta A}{\delta q_k} \right)_{,l} \frac{\delta G}{\delta P_{lk}} - \left(\frac{\delta G}{\delta q_k} \right)_{,l} \frac{\delta A}{\delta P_{lk}} \right] \end{aligned} \tag{19}$$

then the time evolution equations for s, q and P implied by (18) and (19) are of the Maxwell-Cattaneo type as introduced in extended irreversible thermodynamics. The quantities μ_1 and μ_2 in (18) are here constant coefficients and can easily be related to the coefficients appearing in extended irreversible thermodynamics. Preliminarily, we have to prove that $\{A, G\}$ defined by expression (19) is a Poisson bracket. By application

of theorem 1 in Morrison (1983), we see that if μ_1 and μ_2 are independent of the state variables, then the quantity $\{A, G\}$ meets the conditions required to be identified with a Poisson bracket.

Performing integration by parts, equation (19) can be cast into the form

$$\{A, G\} = \frac{1}{V} \int dr \frac{\delta A}{\delta s} \left[-\mu_1 \left(\frac{\delta E}{\delta q_k} \right)_{,k} \right] + \frac{1}{V} \int dr \frac{\delta A}{\delta q_k} \times \left[-\mu_1 \left(\frac{\delta E}{\delta s} \right)_{,k} - \mu_2 \left(\frac{\delta E}{\delta P_{kl}} \right)_{,l} \right] + \frac{1}{V} \int dr \frac{\delta A}{\delta P_{kl}} \left[-\mu_2 \left(\frac{\delta E}{\delta q_k} \right)_{,l} \right]. \tag{20}$$

It follows from expression (17) that the evolution equation (18) for A can be written as

$$\int dr \left(\frac{\delta A}{\delta s} \partial_t s + \frac{\delta A}{\delta q_k} \partial_t q_k + \frac{\delta A}{\delta P_{kl}} \partial_t P_{kl} \right) = \int dr \left[\frac{\delta A}{\delta s} (-\mu_1 e_{q_k,k}) + \frac{\delta A}{\delta q_k} (-\mu_1 e_{s,k} - \mu_2 e_{P_{kl},l}) + \frac{\delta A}{\delta P_{kl}} (-\mu_2 e_{q_k,l}) \right]. \tag{21}$$

Since relation (21) must hold for all A , it is inferred that, by identification of the coefficients of $\delta A/\delta s$, $\delta A/\delta q_k$ and $\delta A/\delta P_{kl}$ respectively,

$$\partial_t s = -\mu_1 (e_{q_k})_{,k} \tag{22}$$

$$\partial_t q_k = -\mu_1 (e_s)_{,k} - \mu_2 (e_{P_{kl}})_{,l} \tag{23}$$

$$\partial_t P_{kl} = -\mu_2 (e_{q_k})_{,l}. \tag{24}$$

Extended irreversible thermodynamics predicts that up to the second-order approximation in the fluxes, one has (Jou *et al* 1988)

$$de = T ds + \frac{\tau_1}{\lambda T} q_k dq_k + \frac{\tau_2}{2\eta} P_{kl} dP_{kl} \tag{25}$$

wherein the non-identified coefficients λ , η are the heat conductivity and the shear viscosity while τ_1 and τ_2 are relaxation times, T is the temperature. In view of the generalised Gibbs relation (25), equations (22)–(24) take the form

$$\partial_t s = -\left(\frac{1}{T} q_k \right)_{,k} \tag{26}$$

$$\tau_1 \partial_t q_k = -\lambda T_{,k} + \beta T^2 \lambda P_{kl,l} \tag{27}$$

$$\tau_2 \partial_t P_{kl} = 2\beta \eta T q_{k,l} \tag{28}$$

at the condition to identify μ_1 and μ_2 as

$$\mu_1 = \frac{\lambda}{\tau_1} \quad \mu_2 = -\frac{2\beta \eta \lambda T^2}{\tau_1 \tau_2} \tag{29}$$

where β is a coefficient appearing in the expression of the entropy flux in extended thermodynamics. By comparison with the linearised Maxwell-Cattaneo type equations derived for instance in Jou *et al* (1988), it is seen that the set (26)–(28) represents the non-dissipative parts of the evolution equations of extended irreversible thermodynamics. Note also that (26) is identical to the entropy conservation law (16) with the entropy flux given by

$$J_k^s = \frac{1}{T} q_k. \tag{30}$$

It is also interesting to notice that the balance law for the energy is of the form

$$\partial_t e = -(q_k - \beta TP_{kl}q_l)_{,k} \tag{31}$$

from which follows that the energy flux contains, besides the classical contribution q_k , an extra term $-\beta TP_{kl}q_l$. In extended thermodynamics, this term is not present in the energy equation but the entropy flux contains, besides q_k/T , an additional term given by $\beta P_{kl}q_l$. To see that there is no contradiction between extended thermodynamics and the theory presented here, let us define a new heat flux q'_k by

$$q'_k = q_k - \beta TP_{kl}q_l. \tag{32}$$

Then the energy law (31) takes the familiar form

$$\partial_t e = -q'_{k,k} \tag{33}$$

while the entropy flux is given by

$$J_k^s = \frac{1}{T} q'_k + \beta P_{kl}q_l \tag{34}$$

in full accord with extended thermodynamics. Expressions (27) and (28) for the evolution of q_k and P_{kl} are unchanged as we have restricted ourselves to the linear approach.

It is worthwhile to stress that one recovers terms like $P_{kl,k}$ and $q_{l,k}$ which are not found in the Maxwell-Cattaneo original relations but which are typical of extended thermodynamics. It must also be pointed out that the generating function has a well-defined meaning as it is identified with the internal energy.

In view to discuss dissipative systems, it is convenient to reformulate the previous results in the entropy representation. If we rewrite the bracket (19) in the entropy representation by using the transformation laws

$$\begin{aligned} \frac{\delta}{\delta s} &\rightarrow s_e^{-1} \frac{\delta}{\delta e}, \quad \frac{\delta}{\delta q_k} \rightarrow \frac{\delta}{\delta q_k} - s_e^{-1} s_{q_k} \frac{\delta}{\delta e} \\ \frac{\delta}{\delta P_{kl}} &\rightarrow \frac{\delta}{\delta P_{kl}} - s_e^{-1} s_{P_{kl}} \frac{\delta}{\delta e} \end{aligned}$$

one obtains

$$\begin{aligned} \{A, G\} = & -\frac{1}{V} \int d\mathbf{r} \mu_1 s_e^{-2} s_{q_k} \left[\left(\frac{\delta A}{\delta e} \right)_{,k} \frac{\delta G}{\delta e} - \left(\frac{\delta G}{\delta e} \right)_{,k} \frac{\delta A}{\delta e} \right] \\ & + \frac{1}{V} \int d\mathbf{r} \mu_2 s_e^{-1} s_{P_{lk}} \left[\left(s_e^{-1} s_{q_k} \frac{\delta A}{\delta e} \right)_{,l} \frac{\delta G}{\delta e} - \left(s_e^{-1} s_{q_k} \frac{\delta G}{\delta e} \right)_{,l} \frac{\delta A}{\delta e} \right] \\ & + \frac{1}{V} \int d\mathbf{r} \mu_1 s_e^{-1} \left[\left(\frac{\delta A}{\delta q_k} \right)_{,k} \frac{\delta G}{\delta e} - \left(\frac{\delta G}{\delta q_k} \right)_{,k} \frac{\delta A}{\delta e} \right] \\ & - \frac{1}{V} \int d\mathbf{r} \mu_2 s_e^{-1} s_{P_{lk}} \left[\left(\frac{\delta A}{\delta q_k} \right)_{,l} \frac{\delta G}{\delta e} - \left(\frac{\delta G}{\delta q_k} \right)_{,l} \frac{\delta A}{\delta e} \right] \\ & - \frac{1}{V} \int d\mathbf{r} \mu_2 s_e^{-1} s_{q_k} \left[\left(\frac{\delta A}{\delta P_{kl}} \right)_{,l} \frac{\delta G}{\delta e} - \left(\frac{\delta G}{\delta P_{kl}} \right)_{,l} \frac{\delta A}{\delta e} \right] \\ & - \frac{1}{V} \int d\mathbf{r} \mu_2 \left[\left(\frac{\delta A}{\delta q_k} \right)_{,l} \frac{\delta G}{\delta P_{lk}} - \left(\frac{\delta G}{\delta q_k} \right)_{,l} \frac{\delta A}{\delta P_{lk}} \right]. \tag{35} \end{aligned}$$

The entropy S is a Casimir functional for the bracket (35). We recall that a functional C is called a Casimir (or distinguished) functional corresponding to a given bracket $\{A, G\}$ if $\{A, C\} = 0$ for all functions A .

After integration by parts and identification of G with the total energy E , the evolution equation (18) for A may be written as

$$\int d\mathbf{r} \left(\frac{\delta A}{\delta e} \partial_t e + \frac{\delta A}{\delta q_k} \partial_t q_k + \frac{\delta A}{\delta P_{kl}} \partial_t P_{kl} \right) = \int d\mathbf{r} \left[\mu_1 (s_e^{-2} s_{q_k})_{,k} \frac{\delta A}{\delta e} - \mu_1 (s_e^{-1})_{,k} \frac{\delta A}{\delta q_k} - \mu_2 (s_e^{-2} s_{P_{kl}} s_{q_r})_{,k} \frac{\delta A}{\delta e} + \mu_2 (s_e^{-1} s_{P_{kl}})_{,l} \frac{\delta A}{\delta q_k} + \mu_2 (s_e^{-1} s_{q_k})_{,l} \frac{\delta A}{\delta P_{kl}} \right]. \tag{36}$$

The time evolution equations for the set e, q_k, P_{kl} derived from (36) read:

$$\partial_t e = \mu_1 (s_e^{-2} s_{q_k})_{,k} - \mu_2 (s_e^{-2} s_{P_{kl}} s_{q_l})_{,k} \tag{37}$$

$$\partial_t q_k = -\mu_1 (s_e^{-1})_{,k} + \mu_2 (s_e^{-1} s_{P_{kl}})_{,l} \tag{38}$$

$$\partial_t P_{kl} = \mu_2 (s_e^{-1} s_{q_k})_{,l}. \tag{39}$$

By taking for μ_1 and μ_2 the same values as in (29), one finds that (37)–(39) reduce to the same evolution equations (31), (27) and (28) as before. Since the entropy is now the generating function, it is automatically conserved. Indeed it is directly checked that

$$\partial_t S = - \left(\frac{1}{T} q_k \right)_{,k}. \tag{40}$$

3.2. Dissipative evolution

In dissipative systems, conservation of energy is still preserved but the entropy is a growing function of time obeying the evolution equation

$$\partial_t S = -J'_{k,k} + \sigma' \tag{41}$$

wherein σ' is the non-negative rate of entropy production per unit volume:

$$\sigma' \geq 0. \tag{42}$$

Dissipation is incorporated in equations (38) and (39) by following the same procedure as in section 2. One introduces a dissipative potential Φ , which is a real-valued functional of $s_{q_k}, s_{P_{kl}}$, and eventually their gradients; Φ is assumed to comply with the same conditions of minimum and convexity as presented at the end of section 2. As a consequence of these properties, it is suggested (Grmela 1984) to relate Φ to the rate of entropy production by means of

$$\sigma' \stackrel{\text{def}}{=} s_{q_k} \frac{\delta \Phi}{\delta s_{q_k}} + s_{P_{kl}} \frac{\delta \Phi}{\delta s_{P_{kl}}} + s_{q_{k,l}} \frac{\delta \Phi}{\delta (s_{q_{k,l}})} + s_{P_{kl,m}} \frac{\delta \Phi}{\delta s_{P_{kl,m}}}. \tag{43}$$

The bracket formulation in presence of dissipation is now modified as follows:

$$\frac{dA}{dt} = \frac{1}{V} \{A, G\} + \frac{1}{V} [A, G] \tag{44}$$

wherein the non-dissipative part $\{A, G\}$ is still given by (35) while the dissipative contribution $[A, G]$ is such that

$$[A, G] = \frac{1}{2V} \int d\mathbf{r} \left[A_{q_k} \frac{\delta\Phi}{\delta G_{q_k}} + A_{P_{kl}} \frac{\delta\Phi}{\delta G_{P_{kl}}} + (A_{q_k})_{,l} \frac{\delta\Phi}{\delta (G_{q_k})_{,l}} + A_{P_{kl,m}} \frac{\delta\Phi}{\delta (G_{P_{kl}})_{,m}} \right]. \tag{45}$$

It is directly checked that the evolution equations implied by the bracket formulation (44) can be written as

$$\partial_t e = \mu_1 (s_e^{-2} s_{q_k})_{,k} - \mu_2 (s_e^{-2} s_{P_{kl}} s_{q_l})_{,k} \tag{46}$$

$$\partial_t q_k = -\mu_1 (s_e^{-1})_{,k} + \mu_2 (s_e^{-1} s_{P_{kl}})_{,l} + \frac{\delta\Phi}{\delta s_{q_k}} - \left(\frac{\delta\Phi}{\delta (s_{q_k})_{,l}} \right)_{,l} \tag{47}$$

$$\partial_t P_{kl} = \mu_2 (s_e^{-1} s_{q_k})_{,l} + \frac{\delta\Phi}{\delta s_{P_{kl}}} - \left(\frac{\delta\Phi}{\delta (s_{P_{kl}})_{,m}} \right)_{,m}. \tag{48}$$

In the case that Φ is a quadratic function of s_{q_k} and $s_{P_{kl}}$, a particular form for Φ is

$$\Phi = \frac{1}{2} \frac{\lambda T^2}{\tau_1^2} s_{q_k} s_{q_k} + \frac{\eta T}{\tau_2^2} s_{P_{kl}} s_{P_{kl}}. \tag{49}$$

Relations (46)–(48) are then exactly the evolution equations derived in the linear version of extended thermodynamics (Jou *et al* 1988), namely

$$\partial_t e = -(q_k - \beta T P_{kl} q_l)_{,k} \tag{50}$$

$$\tau_1 \partial_t q_k = -\lambda T_{,k} + \beta \lambda T^2 P_{kl,l} - q_k \tag{51}$$

$$\tau_2 \partial_t P_{kl} = 2\beta \eta T q_{k,l} - P_{kl}. \tag{52}$$

The absence of terms in $v_{k,l}$ is a consequence of the assumption that the system under consideration is at rest.

If the functional s is chosen to depend in addition on the gradients $q_{k,l}$ and $P_{kl,m}$, meaning that a non-local dependence is introduced, then everything remains the same except that we have to replace the Volterra functional derivatives $\delta/\delta q_k$, $\delta/\delta P_{kl}$ by the variational derivatives $\delta/\delta q_k - (\delta/\delta q_{k,l})_{,l}$, $\delta/\delta P_{kl} - (\delta/\delta P_{kl,m})_{,m}$.

4. Conclusions

Two kinds of arguments can be used to justify the validity of the time evolution equations of extended irreversible thermodynamics. First, it is the comparison of their consequences with experimental observations; second, it is their link with some more fundamental microscopic description. Both of these arguments may be found in Jou *et al* (1988). In the present paper, we add new arguments in favour of extended thermodynamics. We show that, in common with other modes of description such as classical mechanics, kinetic theory, electromagnetism, classical irreversible thermodynamics, the basic equations of extended thermodynamics (at least for an incompressible fluid at rest) share the property to possess a Hamiltonian structure. Moreover, the dynamical equations are generated by a functional that has the physical meaning of a free energy. In other words, we have seen that the systematic way followed in various branches of physics to derive the set of basic dynamical equations is also applicable within the context of extended irreversible thermodynamics.

It is also worth emphasising that the entropy function, used in extended thermodynamics is the same quantity that arises in the generalised Hamiltonian formalism in the form of the generating functional. This comparison provides a supplementary confirmation of the well-foundedness of the entropy introduced in extended thermodynamics.

Concerning comparison with experimental data, it must be recalled that a generalised Hamiltonian structure guarantees that the solutions of the corresponding dynamical equations agree with the equilibrium thermodynamic experience (i.e. the observation that systems that are isolated from any external influence reach, as time goes to infinity, a state at which they are well described by equilibrium thermodynamics). Another advantage of this Hamiltonian structure is that the mathematical methods that were developed in the general context of Hamiltonian systems now also become applicable within the framework of extended irreversible thermodynamics.

References

- Arnold V I 1965 *Dokl. Akad. Nauk. Math.* **162** 773
- Callen M B 1985 *Thermodynamics, an introduction to thermostatics* 2nd edn (New York: Wiley)
- Casas J, Jou D and Lebon G 1984 (eds) *Recent Developments in Nonequilibrium Thermodynamics (Lecture Notes in Physics 199)* (Berlin: Springer)
- Castillo L and Garcia-Colin L 1986 *Phys. Rev. B* **33** 4944
- Clebsh A 1895 *J. Reine Angew. Math.* **56** 1
- De Groot S and Mazur P 1962 *Non Equilibrium Thermodynamics* (Amsterdam: North-Holland)
- Dzyaloshinskii I E and Volovick G F 1980 *Ann. Phys.* **125** 67
- Edelen D 1972 *Int. J. Eng. Sci.* **10** 481
- Grmela M 1984 *Contemp. Math.* **28** 125
- 1986 *Physica D* **21** 179
- 1988 Thermodynamical Structure of Dynamical Theories *Report Ecole Polytechnique Montreal*
- 1989 *J. Phys. A: Math. Gen.* **20** 4375-94
- Holm D, Marsden J, Ratiu T and Weinstein A 1985 *Phys. Rep.* **123** 1
- Iwinski Z and Turski L 1976 *Lett. Appl. Sci. Eng.* **10** 174
- Jou D, Casas-Vazquez J and Lebon G 1988 *Rep. Prog. Phys.* **51** 1105
- Kaufman A 1984 *Phys. Lett.* **100A** 419
- Lebon G and Clout A 1988 *J. Non-Newtonian Fluid Mech.* **28** 61
- 1989 *Wave Motion* **11** 23
- Lebon G, Dauby P, Palumbo A and Valenti G 1990 *Rheol. Acta* **29** 127
- Moreau J 1970 *C. R. Acad. Sci., Paris* **271** 608
- Morrison P 1980 *Phys. Lett.* **80A** 383
- 1983 *Mathematical methods in hydrodynamics and integrability in related dynamical systems (AIP Conf. Proc. 88)* ed M Tabor and Y M Trebe (New York: AIP)
- Perez-Garcia C, Casas-Vazquez J and Lebon G 1989 *J. Polym. Sci.* **B 27**
- Prigogine I 1961 *Introduction to Thermodynamics of Irreversible Processes* (New York: Interscience)
- Valesco R and Garcia-Colin L 1983 *J. Non-Equil. Thermodyn.* **8** 85