Mesoscopic derivation of hyperbolic transport equations

M. A. Olivares-Robles and L. S. García-Colín*
Departamento de Física, Universidad Autónoma Metropolitana-Iztapalapa 09340, Iztapalapa Distrito Federal, Mexico
(Received 15 April 1994)

In this paper we present a derivation of the hyperbolic type of Fokker-Planck equations governing the dynamics of the numerical values associated to a set of observables of a many body system. The ensuing transport equations for the appropriate averages of such variables, namely the gross variables, are also obtained. In both cases we simply extend the ideas set forth by M. S. Green in his work on the statistical mechanics of transport phenomena [J. Chem. Phys. **20**, 1281 (1952)]. These types of equations have been recently used to cope with a large class of transport phenomena. We thus discuss at length the generalized thermodynamic frame to which these equations belong and compare the results with other recent approaches to irreversible thermodynamics.

PACS number(s): 05.40.+j, 05.70.Ln, 05.60.+w

I. INTRODUCTION

In recent years a strong interest has arisen to cope with transport processes using hyperbolic type differential equations, sometimes also referred to as the telegraphist equations. This trend contrasts with the ordinary transport equations of the parabolic type which stem from the postulates of linear irreversible thermodynamics (LIT). It appears that the first derivation of a telegraphist equation in connection with diffusion type processes originates in the continuum approximation to the evolution equation describing a persistent random walk [1]. In this context, it has been afterwards applied to a wide variety of situations related to this problem. A very recent and pertinent review of all these efforts may be found in the work by Masoliver, Porrá, and Weiss [2–4]. In a rather different context, it has been recently pointed out that a telegraphist type transport equation leads to an "almost exact" interpretation of generalized hydrodynamics [5]. In solid state physics a rather interesting use of this type of equations is found in the study of dispersion and tunneling of electrons in one dimension leading to a first principles quantum mechanical interpretation of the Landauer effect [6,7]. The properties of solutions to the telegraphist type equations as well as their relationship to nonequilibrium properties of systems undergoing irreversible processes have also been studied in detail [8,9].

From a phenomenological point of view the telegraphist transport equation is readily obtained when an ordinary conservation equation, mass, momentum, energy, etc. is supplemented by a constitutive equation of the Maxwell-Cattaneo-Vernotte (MCV) type [10,11]. The main feature of the resulting equation is that it predicts a propagation of the corresponding perturbation with a finite velocity thus solving the old problem inherent in LIT, parabolic type equations lead to infinite velocities. What is completely lacking in the literature is a first principles derivation of hyperbolic type transport equations. Buried in this derivation lies also the question related to the type of irreversible thermodynamics to which these equations belong, a theory that clearly goes beyond the domain of LIT.

The purpose of this paper is to show how using the pioneering ideas introduced by Green in 1952 on the mesoscopic approach to the theory of irreversible processes [12,13] one can very easily derive telegraphist like equations. In fact, one first obtains Fokker-Planck type hyperbolic equations for the probability amplitudes describing the motion of the dynamical variables, and then, after appropriate averaging one obtains hyperbolic equations for their conditional averages, namely, the transport equations. With these results one is further capable of setting the mesoscopic basis of what we shall here refer to as a generalized irreversible thermodynamics which has many common features to the theory now referred to as extended irreversible thermodynamics (EIT) but it is not identical to it.

The paper is divided as follows: In Sec. II we will briefly summarize Green's ideas and argue how by correctly interpreting the time interval required to specify a change between a dynamical variable one can easily derive a hyperbolic type Fokker-Planck equation. The ways in which these results differ from those obtained by Green are discussed. In Sec. III we develop the full thermodynamical formalism that arises from the results of Sec. II and we leave for Sec. IV some pertinent concluding remarks.

II. THE GENERALIZED FOKKER-PLANCK EQUATION

We start from the premise that one can identify a set of observables in the system each one of which is represented by a phase space function $A(\Gamma,t)$, where Γ stands for the position in phase space $\Gamma\equiv(\mathbf{x},\mathbf{p})$ and t for time. Therefore, the vector $\mathbf{A}(\Gamma,t)=\{A_i(\Gamma,t),\ i=1,\ldots,r\}$ stands for the r observables in the system. Each observation performed on the system associates a number a_i with a certain error Δa_i to each observable so that

*Also at el Colegio Nacional, Luis González Obregón 23, 06020, Mexico Distrito Federal, Mexico.

$\mathbf{a}(t)=\{a_i(t)|a_i(t)\le A_i(\Gamma,t)\le a_i+\Delta a_i\}$ is the vector associated to each observation [14]. The set of values for **a** are now regarded as random processes and, moreover, we assume that the vector **A** represents a complete set of observables [12]. The average values of the **a** variables to be defined later are known as the gross variables for the system.

If we denote by $W(a_k,t+\tau_k)$ the probability that an event specified by the vector a_k occurs at a certain time $t+\tau_k$, then by the standard Chapman-Kolmogoroff equation [15] written in Chandrasekhar's form [16], we know that (see Appendix A)

$$W(a_k,t+\tau_k)=\int W(a_k-\Delta a_k,t)W(\Delta a_k,\tau_k)d(\Delta a_k)\ , \tag{1}$$

where Δa_k is the change of the observables a_k in time τ_k, $W(a_k-\Delta a_k,t)$ the probability that a_k has the value $a_k-\Delta a_k$ at time t and $W(\Delta a_k,\tau_k)$ the probability that the change Δa_k occurs in time τ_k; also, k runs from $1,\ldots,r$, the number of observables in the system. The next step to be undertaken is the crucial one in this whole analysis. The way in which one handles τ_k has become a rather controversial and debatable point in almost any derivation of a differential Fokker-Planck equation from Eq. (1). Indeed, let us recall that going as far back as Einstein's work on this question [17], τ_k is first assumed to be a finite time, small compared with a macroscopic, hydrodynamic time but large compared with a microscopic one. τ_k, however, must be long enough to assure that the events $a_k-\Delta a_k$ and a_k are independent. In the usual analysis of these derivations, the limit $\tau_k\to 0$ is taken without any further arguments [18]. As Fürth [19], Kirkwood [20], and others have repeatedly pointed out, this procedure is inconsistent. In fact one can even show that in order that the process governing the dynamics in a space is Markovian, τ_k must be strictly finite [21].

After these remarks we proceed with our analysis of Eq. (1) expanding all quantities there appearing in powers of Δa_k and τ_k. If we now keep terms up to powers in τ_k^2, and in $(\Delta a_k)^2$ and further, not to violate Pawula's theorem [22] we assume that all the moments of the transition probability $W(\Delta a_k,\tau_k)$ of order $n\ge 3$ vanish, we arrive at the result that

$$\begin{aligned}\frac{\partial W}{\partial t}\tau_k+\frac{\partial^2 W}{\partial t^2}\tau_k^2=\int\Bigg\{&-\sum_i\frac{\partial W}{\partial a_i}\Delta a_i W(\Delta a_k,\tau_k)+\frac{1}{2}\sum_{i,j}\frac{\partial^2 W}{\partial a_i\partial a_j}\Delta a_i\Delta a_j W(\Delta a_k,\tau_k)\\&-\sum_i W(a_k,t)\frac{\partial W(\Delta a_k,\tau_k)}{\partial a_i}\Delta a_i+\sum_{i,j}\frac{\partial W}{\partial a_i}\frac{\partial W(\Delta a_k,\tau_k)}{\partial a_j}\Delta a_i\Delta a_j\\&+\frac{1}{2}\sum_{i,j}W(a_k,t)\frac{\partial^2 W(\Delta a_k,\tau_k)}{\partial a_i\partial a_j}\Delta a_i\Delta a_j\Bigg\}d(\Delta a_k)\ ,\quad k=1,\ldots,r\ ,\end{aligned} \tag{2}$$

where use has been made of the fact that

$$\int W(\Delta a_k,\tau_k)d(\Delta a_k)=1$$

and $d(\Delta a_k)$ stands for $d(\Delta a_1)d(\Delta a_2)\cdots d(\Delta a_r)$.

Defining the first two moments of $W(\Delta a_k,\tau_k)$ as

$$\langle\Delta a_i\rangle=\int\Delta a_i W(\Delta a_k,\tau_k)d(\Delta a_k)\ , \tag{3a}$$

$$\langle\Delta a_i\Delta a_j\rangle=\frac{1}{2}\int\Delta a_i\Delta a_j W(\Delta a_k,\tau_k)d(\Delta a_k)\ , \tag{3b}$$

after slight rearrangements Eq. (2) may be rewritten as

$$\tau_k^2\frac{\partial^2 W}{\partial t^2}+\tau_k\frac{\partial W}{\partial t}=-\sum_i\frac{\partial}{\partial a_i}\{W\langle\Delta a_i\rangle\}+\sum_{i,j}\frac{\partial}{\partial a_i}\frac{\partial}{\partial a_j}\{W\langle\Delta a_i\Delta a_j\rangle\}\ , \tag{4}$$

or dividing both members by τ_k,

$$\tau_k\frac{\partial^2 W}{\partial t^2}+\frac{\partial W}{\partial t}=\sum_i\frac{\partial}{\partial a_i}\left\{-\bar{V}_i(a_k)W+\sum_j\frac{\partial}{\partial a_j}\bar{\xi}_{ij}(a_k)W\right\}\ , \tag{5}$$

where,

$$\bar{V}_i(a_k)=\frac{\langle\Delta a_i\rangle}{\tau_k};\quad\bar{\xi}_{ij}(a_k)=\frac{\langle\Delta a_i\Delta a_j\rangle}{\tau_k}\ . \tag{6}$$

Equations (5) and (6) are the main result of this paper. They are similar in structure but of different content as those derived by Green in his original paper [12]. The left hand side contains a second-order time derivative of the probability amplitude $W(a_k,t+\tau_k)$ and most important, the **a**-dependent quantities $\bar{V}_i(a_k)$ and $\bar{\xi}_{ij}(a_k)$ do not require to be evaluated in the limit when $\tau_k\to 0$. Indeed Eq. (5) is completely independent of this assumption and the only reason for the vanishing of higher-order terms in τ_k and in (Δa_k) is, as mentioned before, the consistency requirement imposed by Pawula's theorem. It is needless to emphasize that Eq. (5) is now a hyperbolic type Fokker-Planck equation from which we expect to be able to derive hyperbolic type transport equations. This is the subject of another section.

To finish with the discussion regarding the content of Eq. (5) we now evaluate the coefficients of Eqs. (6) for finite times. This process is considerably simplified by noticing that following steps identical to those used by Green, Eqs. (6) may be rewritten as follows,

$$\langle \Delta a_i \rangle = \langle v_i \rangle \tau_k + \frac{1}{\omega(\mathbf{a})} \sum_j \frac{\partial}{\partial a_j} \omega(\mathbf{a}) \int_0^{\tau_k} d\tau_1 \int_{-\tau_1}^0 d\sigma \langle v_i v_j(\sigma) \rangle \tag{7}$$

and

$$\langle \Delta a_i \Delta a_j \rangle = \int_0^{\tau_k} d\tau' \int_0^{\tau'} ds [\langle v_i v_j(\tau'-s) \rangle + \langle v_j v_i(\tau'-s) \rangle] , \tag{8}$$

where $\omega(\mathbf{a})\Delta \mathbf{a}$ is the volume in $\mathbf{a}$ space and $v_i(\sigma)$ is defined through the obvious relation, $a_i(\Gamma_{\tau_k}) - a_i(\Gamma_0) = \int_0^{\tau_k} v_i(\Gamma_\sigma) d\sigma$, $v_i(\Gamma_\sigma)$ is the speed with which the phase space point Γ travels in phase space. Here $\omega(\mathbf{a})\Delta\mathbf{a}$ stands for $\omega(a_k)\Delta a_k$, $k=1,\ldots,r$.

To undertake the last step of the calculation we need to evaluate the integrals appearing in Eqs. (7) and (8) taking all contributions up to order τ_k^2. This task was accomplished some years ago by one of us [13] so we shall skip all clumsy details and refer the reader to the original source. To proceed with the calculation we use the already established properties of the correlation matrix $\langle v_i v_j(\sigma) \rangle$ [12], namely,

(a) $\langle v_i v_j(\sigma) \rangle = \langle v_j v_i(-\sigma) \rangle$,

(b) $\lim_{\sigma \to \infty} \langle v_i v_j(\sigma) \rangle = \langle v_i \rangle \langle v_j \rangle$,

(c) $\int_0^{\tau_k} d\sigma [\langle v_i v_j(\sigma) \rangle - \langle v_i \rangle \langle v_j \rangle] = \xi_{ij}(a_k)$.

Notice that contrary to Green's procedure, the upper limit of the integral in (c) is τ_k, *not* infinity. Now, it is easy to see that

$$\begin{aligned} \mathcal{J} &\equiv \int_0^{\tau_k} d\tau_1 \int_0^{\tau_1} d\sigma \langle v_i v_j(\sigma) \rangle \\ &= \tau_k \int_0^{\tau_k} d\sigma (1-\sigma/\tau_k) \langle v_i v_j(\sigma) \rangle . \end{aligned}$$

Next, adding and subtracting $\langle v_i \rangle \langle v_j \rangle$ from the right hand side of this expression using conditions (b) and (c) and noticing that $\sigma/\tau_k \simeq 0$ since $\tau_k \gg \sigma$ one gets that

$$\mathcal{J} = \tau_k \xi_{ij}(a_k) + \tfrac{1}{2}\tau_k^2 \langle v_i \rangle \langle v_j \rangle ,$$

which together with condition (a) leads to the result that

$$\langle \Delta a_i \rangle = \langle v_i \rangle \tau_k + \frac{1}{\omega(\mathbf{a})} \sum_j \frac{\partial}{\partial a_j} \omega(\mathbf{a}) [\tau_k \xi_{ij}(a_k) + \tfrac{1}{2}\tau_k^2 \langle v_i \rangle \langle v_j \rangle] ,$$

which substituted in Eq. (6) gives

$$\bar{V}_i(a_k) = \langle v_i \rangle + \frac{1}{\omega(\mathbf{a})} \sum_j \frac{\partial}{\partial a_j} \omega(\mathbf{a}) [\xi_{ij}(a_k) + \tfrac{1}{2}\tau_k \langle v_i \rangle \langle v_j \rangle] ,$$

$$\bar{V}_i(a_k) = \langle v_i \rangle + \frac{1}{\omega(\mathbf{a})} \sum_j \frac{\partial}{\partial a_j} \omega(\mathbf{a}) C_{ij}(a_k, \tau_k) , \tag{9}$$

where

$$C_{ij}(a_k,\tau_k) = \xi_{ij}(a_k) + \tfrac{1}{2}\tau_k \langle v_i \rangle \langle v_j \rangle . \tag{10}$$

Proceeding in a similar way we get that

$$\bar{\xi}_{ij}(a_k) = \tfrac{1}{2}[C_{ij}(a_k,\tau_k) + C_{ji}(a_k,\tau_k)] = C_{ij}(a_k,\tau_k) , \tag{11}$$

since C_{ij} is symmetric under the exchange of indices i and j [23].

If we now substitute Eqs. (10) and (11) into Eq. (5) we find that

$$\tau_k \frac{\partial^2 W}{\partial t^2} + \frac{\partial W}{\partial t} = \sum_{i=1} \frac{\partial}{\partial a_i} \left\{ - \left[\langle v_i \rangle + \frac{1}{\omega(\mathbf{a})} \sum_j \frac{\partial}{\partial a_j} \omega(\mathbf{a}) C_{ij}(a_k,\tau_k) \right] W + \sum_j \frac{\partial}{\partial a_j} C_{ij}(a_k,\tau_k) W \right\} . \tag{12}$$

We want to emphasize that the main difference between Eq. (12) and the one derived by Green [see Eq. (30), Ref. [12]] lies not only on the fact that by keeping τ_k finite the second order in time derivative in W appears in the left hand side but also that the quantities $C_{ij}(a_k,\tau_k)$, here playing the role of generalized transport coefficients satisfying Onsager's reciprocity relations, are also state [($\mathbf{a}$) dependent] and time dependent. In this sense this result is in agreement with the early work of Kirkwood in which he computed the friction coefficient in a fluid [20] and with more recent work of Hurley and Garrod [24] who generalized Onsager's reciprocity theorem to state and time dependent transport coefficients. A broader discussion of the implications behind these ideas has been reported earlier [25,26].

III. PHENOMENOLOGICAL IMPLICATIONS

In this section we undertake the task of deriving the most relevant phenomenological implications arising from Eq. (12). We begin with the corresponding equations of motion that are obeyed by the average values $\langle a_k \rangle$ associated to each of the variables a_k. These averages are defined as

$$\langle a_k \rangle = \int a_k W(a_k^{(0)}, t_0 | a_k, t) d\mathbf{a} ,$$

where $d\mathbf{a} = \prod_{i=1}^r da_i$ and $W(a_k^{(0)}, t_0 | a_k, t)$ is the conditional probability that the event characterized by a_k occurs at time t provided that at an earlier time t_0 it had the value $a_k^{(0)}$. Multiplying Eq. (12) by a_k and integrating by parts (see Appendix B) we get that,

$$\tau_k \frac{d^2 \langle a_k \rangle}{dt^2} + \frac{d\langle a_k \rangle}{dt} = \int \left\{ \langle v_k \rangle + \sum_j C_{kj}(a_k,\tau_k) \frac{\partial \ln \omega(\mathbf{a})}{\partial a_j} + \sum_j \frac{\partial}{\partial a_j} C_{kj}(a_k,\tau_k) \right\} W d\mathbf{a} . \tag{13}$$

If we now assume that the conditional probability W is sharply peaked around the mean values $\langle a_k \rangle$, Eq. (13)

reduces to a set of ordinary differential equations, namely,

$$\tau_k \frac{d^2\langle a_k \rangle}{dt^2} + \frac{d\langle a_k \rangle}{dt} = \left[\langle v_k + \sum_j C_{kj}(a_k,\tau_k) \frac{\partial \ln\omega(\mathbf{a})}{\partial a_j} + \sum_j \frac{\partial}{\partial \mathbf{a}_j} C_{kj}(a_k,\tau_k) \right]_{\langle a_i \rangle \cdots \langle a_r \rangle} , \tag{14}$$

where, we emphasize, τ_k is the characteristic time associated to the number variable a_k.

The set of Eqs. (14) for $\langle a_k \rangle$ $k=1,\ldots r$, r being the number of observables, are the sought transport equations which as expected, are of the hyperbolic type differential equations. If $\tau_k \to 0$ they reduce to those derived by Green [12]. It is now a straightforward step to convince oneself that all the steps given in Green's work to show that the equilibrium solution to Eq. (14) has to be of the form $\omega(\mathbf{A})\Psi[E(\mathbf{A})]$, where $\Psi[E(\mathbf{A})]$ is determined by the distribution of energy $H(\Gamma)=E[\mathbf{A}(\Gamma)]$ where H is the system's Hamiltonian, follow at once. Thus, for Eq. (14) the equilibrium solutions exists as has been also pointed out in specific cases treated in the literature [8,9].

Moreover, to study the significance of Eqs. (14), let us introduce following Onsager, the fluxes associated to the gross variables $\langle a_k \rangle$ by

$$\frac{d\langle a_k \rangle}{dt} = J_k ,$$

so that Eq. (14) now reads as

$$\tau_k \frac{dJ_k}{dt} + J_k = \langle v_k \rangle + \sum_j C_{kj}(a_k,\tau_k) \frac{\partial \ln\omega(\mathbf{a})}{\partial a_j} + \sum_j \frac{\partial}{\partial a_j} C_{kj}(a_k,\tau_k) , \tag{15}$$

where we omit the explicit notation that the right hand side must be evaluated at the expectation values $\langle a_k \rangle$. We first notice that if $\tau_k \to 0$, $\langle v_k \rangle$ is neglected since as Green proved it gives no contributions to an irreversible process, C_{kj} which is now identical to ξ_{kj} according to Eq. (10) is assumed to be constant and the force conjugated to J_k is defined as $\partial S/\partial a_k$, where S is the local nonequilibrium entropy given by $S=k_B \ln\omega(\mathbf{a})$ according to Boltzmann's definition, Eq. (15) reduces to the well known flux-force relations of linear irreversible thermodynamics (LIT)

$$\frac{d\langle a_k \rangle}{dt} = J_k = \sum_{j=1}^{r} \xi_{jk} X_j , \tag{16}$$

where k_B, Boltzmann's constant is absorbed in the definition of ξ_{jk}. Since $\xi_{jk} = \xi_{kj}$ the correlation or transport matrix ξ_{jk} satisfies Onsager's reciprocity condition. It is then clear that the transport equations given by (15), even ignoring the term $\langle v_k \rangle$ are more general than the linear relations of LIT.

It is worth noticing, that Eqs. (15) are of the so called Maxwell-Vernotte-Cattaneo type when τ_k is interpreted as the nonzero relaxation time of the flux J_k. As mentioned in the Introduction these equations are very successful in eliminating the infinite speed propagation of the disturbance produced in a system by an irreversible process. Since the coefficients $C_{kj}(a_k,\tau_k)$ are symmetric, one can state that the underlying thermodynamic theory to which these equations belong still satisfies the Onsager reciprocity condition in a more general form that the one implied by Eq. (16). If we still maintain the definition of X_k, the thermodynamic force associated to J_k, as the derivative of the local nonequilibrium entropy density $k_B \ln\omega(\mathbf{a})$ with respect to $\langle a_k \rangle$, Eq. (15) read as

$$\tau_k \frac{dJ_k}{dt} + J_k = \sum_j C_{kj}(a_k,\tau_k) \frac{1}{k_B} X_j + \sum_j \frac{\partial}{\partial a_j} C_{kj}(a_k,\tau_k) , \tag{17}$$

which may be regarded as the generalization of Eq. (16) consistent with the hyperbolic type transport equations given by Eq. (12). Phenomenological MCV type equations have been used in different formulations of what is now referred to as extended irreversible thermodynamics (EIT) [10,11], but in none of them has an effort been made to somehow incorporate Onsager's reciprocity theorem at least in the context of state and time dependent transport coefficients.

There is a far more difficult question to answer now, namely, the form of the nonequilibrium entropy which is consistent with Eq. (17). In LIT the local equilibrium assumption guarantees that $S=k_B \ln\omega(\mathbf{a})$ is the correct answer and as shown by Green, this leads both to a proof that $S_{\text{eq}} > S$ and that the entropy production is semipositive definite. In our case we have no aprioristic way of choosing the appropriate form for the nonequilibrium entropy since clearly, Eq. (12) indicates that we are dealing with states of the system which are no longer at grips with the local equilibrium assumption. Moreover Eq. (17), as has been largely manifested in EIT [10,11], shows that the fluxes have been raised to the status of independent states variables. Thus we should suspect that the nonequilibrium entropy consistent with these facts ought to be a function of the gross variables $\langle a_k \rangle$ and the fluxes J_k. Inspired by this result, also supported by an exact solution of Boltzmann's equation using the nontruncated moment method developed by Grad [27] we will assume that the nonequilibrium entropy $S(\langle \mathbf{a} \rangle, \mathbf{J})$ is to be of the form [28]

$$\rho S(\langle \mathbf{a} \rangle, \mathbf{J}) = \rho S_{\text{LE}} - \frac{1}{\chi(\mathbf{a})} \sum_l \tau_l J_l J_l , \tag{18}$$

where $S_{\text{LE}} \equiv k_B \ln\omega(\langle \mathbf{a} \rangle)$ is the local equilibrium entropy of LIT, ρ the mass density and $\chi(\langle \mathbf{a} \rangle)$ which we write as χ for short, is a still undetermined quantity that may depend on the gross variables $\langle \mathbf{a} \rangle$. An explicit example of how an expression of the type (18) increases monotonically with time in a system where heat conduction is governed by a hyperbolic transport equation has been recently discussed in the literature [9]. In spite of this we warn the reader that we are by no means claiming that Eq. (18) is neither unique nor the most general form for the entropy. Nevertheless, it leads to rather interesting results as we now show.

Since the time behavior of ρS_{LE} has been carefully analyzed in Green's paper [29], we shall restrict ourselves here to the study of the time behavior of

$$\rho\Delta S \equiv \rho[S(\langle \mathbf{a}\rangle,\mathbf{J})-S_{\text{LE}}(\mathbf{a})] = -\frac{1}{\chi(\mathbf{a})}\sum_l \tau_l J_l J_l \ .$$

Taking its time derivative we get

$$\frac{d}{dt}\rho(\Delta S) = -\frac{1}{\chi(\mathbf{a})}2\sum_l \tau_l J_l \frac{d}{dt}J_l \ , \tag{19}$$

which with the aid of Eq. (12) after some obvious simplifications yields,

$$\frac{d}{dt}\rho(\Delta S) = -\sum_l \frac{2J_l}{\chi(\mathbf{a})}\left[-J_l+\sum_j C_{lj}(a_k,\tau_k)\frac{\partial \ln\omega(\mathbf{a})}{\partial a_j} + \sum_j \frac{\partial}{\partial a_j}C_{lj}(a_k,\tau_k)\right] , \tag{20}$$

the term $\langle v_k\rangle$ being ignored for reasons already mentioned.

Using the definitions of X_j in terms of $\ln\omega(\mathbf{a})$ and rearranging terms in Eq. (20) we finally arrive at the result that

$$\frac{d}{dt}(\rho\Delta S) = \sum_l \frac{2J_l}{\chi(\mathbf{a})}J_l - \sum_l\sum_j 2\frac{C_{lj}(a_k,\tau_k)}{k_B\chi(\mathbf{a})}J_l X_j - \sum_l \frac{2J_l}{\chi(\mathbf{a})}\sum_{i=1}\frac{\partial}{\partial a_i}C_{lj}(a_k,\tau_k) \ . \tag{21}$$

In analogy to the local equilibrium entropy, Eq. (21) can also be written in the form of an entropy balance equation using the following definitions: (i) The entropy flux vector $(\mathbf{J}_s)_j$ (jth component) in **a** space is

$$[\mathbf{J}_s]_j \equiv \sum_l \frac{2}{\chi(\mathbf{a})}J_l C_{lj}(a_k,\tau_k) \ . \tag{22}$$

(ii) The entropy production σ_s is given by

$$\sigma_s \equiv \sum_l \frac{2}{\chi(\mathbf{a})}J_l J_l - \sum_l\sum_j 2\frac{C_{lj}(a_k,\tau_k)}{\chi}J_l X_j \ . \tag{23}$$

It follows at once that by letting $\sum_j(\partial/\partial a_j)$ be the divergence operation in a space, Eq. (21) takes the form

$$\frac{d}{dt}(\rho\Delta S)+\text{div}_{\mathbf{a}}\mathbf{J}_s = \sigma_s \ . \tag{24}$$

The difference between Eqs. (24) and (47) of Ref. [12] for the local equilibrium entropy is that we are no longer able to prove in general that σ_s is semipositive definite. The first term which is quadratic in the fluxes is always non-negative but the sign of the full expression of Eq. (24) is undetermined. For the present time nothing else may be stated from a general point of view. Nevertheless Eqs. (22) and (23) may be compared with other efforts that have been attempted in the literature to extend the concepts of irreversible thermodynamics beyond the linear domain. One interesting feature of Eq. (22) is that it depends only on a linear combination of the physical fluxes multiplied by the generalized transport coefficients. Notice should be made, however, that this is within the spirit of Onsagerian thermodynamics since J_k is defined as the time rate of change of the gross variable $\langle a_k\rangle$. In the many attempts that have been made to combine Grad's moment solution of Boltzmann's equation with the definition of entropy, the entropy flux has nonunique forms depending on how the calculations are performed [27,30]. Thus the structure of the phenomenological equations are also questionable [30]. Here this is not the case although to carry out a more detailed comparison, the results of this paper must be first written in configuration space and not in **a** space. This task is the subject of future work.

As far as Eq. (23) is concerned similar comments are applicable. Even starting from more fundamental principles than those used in this work, to derive the general structure of nonlinear irreversible thermodynamics [31,32] a proof that the entropy production is semipositive definite beyond the linear regime is still lacking. A deeper discussion relating such a methodology to the one presented in this paper is also a subject for future work.

IV. CONCLUDING REMARKS

Here we merely wish to emphasize which are the main results obtained in this work. The central idea is to examine the derivation of the Fokker-Planck type equation of motion that governs the dynamics of a physical system in **a** space, the space associated to the numerical values of the system's observables. This derivation starts from the Chapman-Kolmogoroff integral equation assuming that the **a** variables $\mathbf{a}\equiv(a_1,\ldots,a_s)$ undergo a stationary random Markoff process. The time interval τ_k required for the occurrence of two events a_k and $a_k+\Delta a_k$ is, contrary to standard procedures, not taken to be zero. By consistency with Pawula's theorem only terms of order τ_k^2 and $(\Delta a_k)^2$ are kept in the derivation which leads to a Fokker-Planck type hyperbolic equation. If one then introduces the average values of the a variables, also referred to as gross variables, one is led to transport equations of the hyperbolic or telegraphist type which are now of wide use in many areas of irreversible processes. These results, the main ones of this paper, are given by Eqs. (12) and (17). We also notice that the generalized transport coefficients appearing in them obey Onsager's reciprocity relation and are also state and time dependent.

The second aspect of this work which deserves attention is the fact that the generalized transport equations here derived belong to a thermodynamic frame which lies beyond the one supporting LIT. Indeed, as we have shown in Sec. III the thermodynamic space of states is not the local equilibrium one but contains also the fluxes. This is reminiscent of the theories now referred to as EIT but differs from them in that in our case Onsager's reciprocity theorem still holds true. Nevertheless, the total entropy of the system is shown to obey a balance type equation in which the entropy flux is a linear combination of the fluxes and the entropy production is composed of two terms, one semipositive definite quadratic in the fluxes and a second one which is a bilinear form in the forces, defined *à la* Onsager, and the fluxes. Whether or not this entropy production is always positive definite, remains an open question.

ACKNOWLEDGMENT

M.A.O.R. acknowledges financial support from CONACYT México.

APPENDIX A

Let $W(a_k^{(1)},t_1|a_k^{(2)},\tau_2)$ be the transition probability for the variable $a_k^{(1)}$ at time t_1 to the values $a_k^{(2)}$ at time $t_2>t_1$. The Chapman-Kolmogoroff equation states that

$$W(a_k^{(1)},t_1|a_k^{(3)},t_3)=\int W(a_k^{(1)},t_1|a_k^{(2)},t_2)\times W(a_k^{(2)},t_2|a_k^{(3)},t_3)da_k^{(2)} \quad \text{(A1)}$$

for all values of t_1, t_2, and t_3. If the process is stationary and call $t_3-t_1=t+\tau_k=(t_3-t_2)+(t_2-t_1)$ and let $a_k^{(3)}=a_k$, $a_k^{(2)}=\Delta a_k$, and $a_k^{(1)}=a_k-\Delta a_k$, Eq. (A1) reads as

$$W(a_k-\Delta a_k|a_k,t+\tau_k)=\int W(a_k-\Delta a_k|\Delta a_k,\tau_k)\times W(\Delta a_k,\tau_k|a_k,t+\tau_k)d(\Delta a_k)\ .$$

Omitting the initial state in the transition probabilities in the left hand side and calling for short $W(a_k-\Delta a_k|\Delta a_k,\tau)=W(\Delta a_k,\tau)$ the probability that a_k has the values $a_k-\Delta a_k$ in the time interval τ, the above equation is now

$$W(a_k,t+\tau_k)=\int W(a_k-\Delta a_k,t)W(\Delta a_k,\tau_k)d(\Delta a_k)\ , \quad \text{(A2)}$$

where $W(a_k-\Delta a_k,t)=W(\Delta a_k,\tau_k|a_k,t+\tau_k)$ is the probability that a_k has the value $a_k-\Delta a_k$ at time t. Equation (A2) with $k=1,\ldots,r$ is Eq. (1) in the text.

APPENDIX B

We outline the derivation of Eq. (13) from (12) for a single variable a_k. We first multiply Eq. (12) by a_k, integrate over the whole **a** space to get that

$$\tau_k\frac{d^2\langle a_k\rangle}{dt^2}+\frac{d\langle a_k\rangle}{dt}=\sum_i\int a_k\frac{\partial}{\partial a_i}\{K(i,k)+L(i,k)\}da_k\ , \quad \text{(B1)}$$

where

$$K(i,k)\equiv-\langle v_i\rangle+\frac{1}{\omega}\sum_j\frac{\partial}{\partial a_j}\omega C_{ij}(a_k,\tau_k)W\ , \quad \text{(B2)}$$

$$L(i,k)\equiv\sum_j\frac{\partial}{\partial a_j}C_{ij}(a_k,\tau_k)\ , \quad \text{(B3)}$$

and

$$\langle a_k\rangle=\int a_k W(a_k^{(0)},t_0|a_k,t)d\mathbf{a}\ , \quad \text{(B4)}$$

where $d\mathbf{a}=\prod_{i=1}^r da_i$.

A first integration by parts in (B1) assuming that both $K(i,k)$ and $L(i,k)$ vanish along the boundary of **a** space leads to

$$\tau_k\frac{d^2\langle a_k\rangle}{dt^2}+\frac{d\langle a_k\rangle}{dt}=-\int\left\{-\left[\langle v_k\rangle+\frac{1}{\omega}\sum_j\frac{\partial}{\partial a_j}\omega C_{ij}(a_k,\tau_k)\right]W\,d\mathbf{a}-\int\sum_j\frac{\partial}{\partial a_j}C_{ij}(a_k,\tau_k)W\,d\mathbf{a}\right\}. \quad \text{(B5)}$$

The second integral in the right hand side vanishes if $C_{ij}(a_k,\tau_k)W$ is zero at the **a** boundary so that expanding the term in brackets of the first integral one immediately arrives at Eq. (13) in the text.

[1] S. Goldstein, Q. J. Mech. Appl. Math. **4**, 129 (1951).

[2] J. Masoliver, J. M. Porrá, and G. H. Weiss, Physica A **182**, 593 (1992).

[3] J. Masoliver, J. M. Porrá, and G. H. Weiss, Physica A **193**, 469 (1993).

[4] J. Masoliver, J. M. Porrá, and G. H. Weiss, Phys. Rev. E **48**, 939 (1993).

[5] P. Rosenau, Phys. Rev. E **48**, R655 (1993).

[6] S. Godoy, J. Chem. Phys. **94**, 6214 (1991).

[7] S. Godoy and S. Fujita, J. Chem. Phys. **97**, 5148 (1992).

[8] M. Criado-Sancho and J. E. Llebot, Phys. Lett. A **177**, 323 (1993).

[9] M. Criado-Sancho and J. E. Llebot, Phys. Rev. E **47**, 4104 (1993).

[10] L. S. García-Colín, Rev. Mex. Fis. **34**, 434 (1989).

[11] D. Jou, J. Casas-Vázquez, and G. Lebon, *Extended Irreversible Thermodynamics* (Springer-Verlag, Berlin, 1993).

[12] M. S. Green, J. Chem. Phys. **20**, 1281 (1952).

[13] L. S. García-Colín and J. L. del Río, in *Perspectives in Statistical Physics,* M. S. Green memorial volume, edited by H. J. Ravaché (North-Holland, Amsterdam, 1981), Chap. 4.

[14] The importance of the **a** space in deriving kinetic-type equations has been particularly emphasized by N. G. van Kampen, in *Fundamental Problems in Statistical Mechanics,* edited by E. G. D. Cohen (North-Holland, Amsterdam, 1962), p. 173. Here we are using the same assumptions and terminology as in Green's paper, Ref. [12], Secs. A and B.

[15] See Sec. C in Ref. [12] or any standard book on probability theory.

[16] S. Chandrasekhar, Rev. Mod. Phys. **15**, 1 (1943). Reprinted in *Noise and Stochastic Processes,* edited by N. Wax (Dover, New York, 1954).
[17] A. Einstein, *The Theory of Brownian Movement* (Dover, New York, 1954).
[18] This point is standard in the literature on the derivation of Fokker-Planck equations from the Chapman-Kolmogoroff equation. See however, H. Risken, *The Fokker-Planck Equation,* 2nd ed. (Springer-Verlag, Berlin, 1989).
[19] See Fürth's comments on Einstein's derivation in Ref. [17] loc. cit. p. 97.
[20] J. G. Kirkwood, J. Chem. Phys. **14**, 180 (1946).
[21] J. L. del Río and L. S. García-Colín, Phys. Rev. A **43**, 6657 (1991); Phys. Rev. E **48**, 819 (1993).
[22] R. F. Pawula, Phys. Rev. **162**, 186 (1967), and Risken's book loc. cit. Ref. [18].
[23] This property follows at once from the fact that $\xi_{ij}(\mathbf{a})$ is symmetric under the exchange of indices as shown in Sec. H of Ref. [12].
[24] J. Hurley and C. Garrod, Phys. Rev. Lett. **48**, 1575 (1982).
[25] J. L. del Río and L. S. García-Colín, Phys. Rev. A **30**, 3314 (1984).
[26] L. S. García-Colín and R. F. Rodríguez, Phys. Rev. A **36**, 4945 (1987).
[27] R. M. Velasco and L. S. García-Colín, J. Non-Equilib. Thermodyn. **18**, 157 (1993).
[28] N. G. van Kampen, Physica **25**, 1294 (1959).
[29] In Sec. G of Ref. [12] the non-negative character of the entropy production as well as the increase in entropy law for $S_{\mathrm{LE}}(\mathbf{a})$ are shown to hold true.
[30] R. E. Nettleton, Ann. Phys. (Leipzig) **2**, 490 (1993), and references therein.
[31] L. S. García-Colín, R. Luzzi, and A. Vasconcellos, J. Non-Equilib. Thermodyn. **19**, 24 (1994).
[32] A. Vasconcellos, R. Luzzi, and L. S. García-Colín (unpublished).