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Extensions of Classical Hydrodynamics

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Abstract An abstract dynamical system is formulated from three features extracted from classical hydrodynamics. One its particular realization is then the classical hydrodynamics, other possible realizations are extensions of the classical hydrodynamics. The three features entering the formulation of the abstract dynamical system are the conservation laws, the compatibility with equilibrium thermodynamics, and the compatibility with classical mechanics in the limit of no dissipation. The particular extensions on which we illustrate the process of constructing different realizations are those arising when dealing with fluids in the vicinity of gas-liquid phase transitions (i.e. fluids involving large spatial inhomogeneities and large fluctuations).

Keywords Hydrodynamics · Nonequilibrium thermodynamics · Gas-liquid phase transition · GENERIC

1 Introduction

Classical hydrodynamics has a limited domain of applicability. Polymeric fluids exhibiting viscoelastic flow behavior or fluids in the vicinity of gas-liquid phase transitions are examples of the fluids that lie outside the domain. In the former case it is the presence of polymer macromolecules and in the latter the presence of large spatial inhomogeneities and fluctuations that cause the problem. If the time scale of changes of an internal structure of the fluid (e.g. polymer macromolecules, spatial inhomogeneities and fluctuations) is comparable to the time scale of changes of classical hydrodynamic fields then the classical hydrodynamics has to be coupled to the time evolution of the internal structure. To construct an extended hydrodynamics with an enlarge domain of applicability means thus, first, to recognize the internal structure playing the essential role, and second, to construct in the enlarged state space (consisting of the classical hydrodynamic fields and the extra state variables chosen to characterize the internal structure) the time evolution. There are two strategies that can

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be followed. We can either start on a microscopic level and then gradually reduce the formulation to the level of extended hydrodynamics or we can start on the level of classical hydrodynamics and then try to extend it to a more microscopic level while keeping some of its features that we judge to be important. Both strategies are complementary and should be preferably followed simultaneously. The outcome of the extension can be either one dynamical theory or more appropriately a family of mutually compatible dynamical theories formulated on several different levels of description. The latter formulation is then called a multiscale (or multilevel) model.

The objective of this paper is to explore the method of extension whose point of departure is classical hydrodynamics. As an illustration we formulate an extended hydrodynamics suitable for fluids in the vicinity of gas-liquid phase transition. An extension reported previously in [1] has the same spirit as the one presented below but is done in somewhat different context and is much less complete.

The "holy grail" of classical hydrodynamics is the conservation of mass, momentum and energy. If the state variables are chosen to be the classical hydrodynamic fields, i.e. the local mass, the local momentum, and the local energy, then the requirement of the global conservation provides immediately the framework for the time evolution equations. The framework (that we shall call an abstract dynamical system) consists of the local conservation laws, i.e. the time derivative equals divergence of a flux. The individual features of the fluids are expressed in the fluxes. Their specification is called a constitutive relation. We can also see the search for constitutive relations as a search for different realizations of the abstract dynamical system.

Beside the mass, momentum and energy conservations, what are the other important properties of the governing equations of classical hydrodynamics? We suggest two: compatibility with equilibrium thermodynamics and compatibility with classical mechanics in the limit of no dissipation. We discuss them in the following two paragraphs.

Fluids that are left free of external influences are seen to reach states, called equilibrium states, at which their behavior is seen to be well described by classical thermodynamics. What is the property of solutions expressing this experimental observation and what is the structure of the time evolution equations guaranteeing it? Nonequilibrium thermodynamics has been investigating this question and by doing it contributed to classical hydrodynamics. Roughly speaking, the answer goes as follows: Fluids are seen as being at local equilibrium. Following classical thermodynamics, we introduce a new scalar field, namely the field of local entropy. As in classical thermodynamics where the entropy is a function (called a fundamental thermodynamic relation) of the independent thermodynamic state variables, the local entropy is a function (called a local fundamental thermodynamic relation) of the classical hydrodynamic fields. Their time evolution is restricted by requiring that the entropy never decreases in the course of the time evolution.

Now we turn to the compatibility with classical mechanics. The equation expressing the local conservation of momentum can also be interpreted as a formulation of Newton's law (mass times acceleration equals force). Indeed, Euler has constructed the Euler equation (the equation governing the time evolution of the momentum in the limit of no dissipation) as a continuum version of Newton's law. In classical hydrodynamics this purely mechanical aspect of the time evolution is not used to its full potential. Its main application is in providing a part of the momentum flux with an alternative interpretation (as a force acting on surface).

Our objective is, first, to formulate an abstract dynamical system in which all three properties mentioned above play an equally important role, and second, to construct its various realizations.

2 GENERIC Dynamical System

The abstract dynamical system whose trajectories are guaranteed to agree with the conservations laws and are compatible with thermodynamics and mechanics has been gradually [2–7] extracted from classical hydrodynamics and also from kinetic theories and other mesoscopic theories. It has been called GENERIC in [4, 5]. We shall use this name also here. Keeping the terminology established in hydrodynamics where particular realizations of the local conservation laws are called constitutive relations, we shall use the term GENERIC constitutive relations to denote particular realizations of GENERIC. In this section we recall the formulation of GENERIC. In Sect. 3 we discuss GENERIC constitutive relations corresponding to fluids with large spatial inhomogeneities and fluctuations.

Let x denote the state variables (for example those listed in (11)). The time evolution of x is governed by [2–7]

$$\dot{x} = LE_x + \frac{\partial \Xi}{\partial H_x} \tag{1}$$

called GENERIC. The first term on the right hand side of (1) expresses the compatibility with mechanics, the second the compatibility with thermodynamics. The symbols appearing in (1) have the following meaning.

2.1 Energy

$E(x)$, a real valued function of x, has the physical meaning of the total energy.

By E_x we denote the derivative of E with respect to x. If x involves a field (e.g. the mass density $\rho(\boldsymbol{r})$, $\boldsymbol{r} \in \mathbb{R}^3$ is the position vector) then E is a real valued functional, $E_{\rho(\boldsymbol{r})} = \frac{\delta E}{\delta \rho(\boldsymbol{r})}$ is a function of $\boldsymbol{r}$. By the symbol δ/δ we denote the Volterra functional derivative. In order to simplify the notation we shall write hereafter E_ρ instead of $E_{\rho(\boldsymbol{r})}$.

2.2 Eta-function

$H(x)$ is called an eta-function. It plays the role of the function often called a nonequilibrium entropy. Because of the multitude of meanings that have been associated in the past with the name “nonequilibrium entropy”, we do not use it in the abstract formulation. In the particular case when (1) represents the Boltzmann kinetic equation, the eta-function H is exactly the Boltzmann H-function. In the abstract formulation we use the same symbol but read H as eta.

2.3 Kinematics

The equation

$$\dot{x} = LE_x \tag{2}$$

is the mathematical expression of the compatibility of the time evolution of x with mechanics. To see it, we consider first (2) in the particular case of classical mechanics of particles, i.e. for $x = (q, p)$, where q are position vectors and p the momenta of the particles. Hamiltonian reformulation of Newton’s equations takes the form of (2) where $L = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ and $E(q, p)$ is the energy. The operator L, hereafter called a Poisson bivector, transforms a covector (a gradient of a potential) into a vector and expresses kinematics of the state variables (q, p). We thus see that in this particular example (2) expresses indeed the classical mechanics.

It has been found useful in classical mechanics to reformulate (2) into another form. Having L, we construct a bracket

$$\{A, B\} = \langle A_x, LB_x\rangle \tag{3}$$

where A and B are sufficiently regular real valued functions of x, $\langle , \rangle$ denotes the inner product. The equation (3) defines the bracket for given L and conversely, (3) defines L if the bracket is given. For $x = (q, p)$ and L given in the previous paragraph, we have $\{A, B\} = A_q B_p - B_q A_p$. It is easy to verify that this bracket is a Poisson bracket, i.e. $\{A, B\} = -\{B, A\}$, and the Jacobi identity $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$ holds (A, B, C are sufficiently regular real valued functions of (q, p)). Moreover, we note that L is nondegenerate, i.e. $\{A, B\} = 0$ for all A implies $B = constant$. Having the Poisson bracket, the time evolution equation (2) can now be also written as

$$\dot{A} = \{A, E\} \quad \text{holds for all } A \tag{4}$$

Now we turn to another particular case, namely to the case of classical hydrodynamics, i.e. $x =$ *classical hydrodynamic fields*. Clebsch in [8] has asked the following question: Euler's equation is a continuum version of Newton's law (mass times acceleration equals force), what is its Hamiltonian formulation? His answer given in [8] (reformulated into the form introduced later in [9]) is again (2) with E being the energy and L being a Poisson bivector. The bracket (3) corresponding to the Clebsch reformulation of the governing equations of classical hydrodynamics (written explicitly in Sect. 3.3) is again a Poisson bracket (i.e. it is antisymmetric and the Jacobi identity holds) but it is degenerate: $\{A, H\} = 0$ and $\{A, M\} = 0$ for all A. By $M(x)$ we denote the total mass.

It has been observed that the nondissipative part of the time evolution in the Boltzmann kinetic theory and in many other mesoscopic theories is governed by equations that can all be cast into the form of (2). In this paper we are exploring extensions of classical hydrodynamics that share with the classical hydrodynamics the form (2) of their nondissipative part of the time evolution.

2.4 Dissipation

$\Xi(H_x)$, called a dissipation potential, is a sufficiently regular real valued function of H_x satisfying the following properties: (i) $\Xi(0) = 0$, Ξ reaches its minimum at 0, (iii) Ξ is concave in a neighborhood of 0, and (iv) Ξ is degenerate: $\langle E_x, \frac{\partial \Xi}{\partial H_x}\rangle = 0$, $\langle M_x, \frac{\partial \Xi}{\partial H_x}\rangle = 0$.

2.5 Properties of Solutions of (1)

The properties required from E, M, H, L, Ξ introduced above imply that solutions to (1) have the following properties:

(i)

$$\frac{dM}{dt} = 0; \qquad \frac{dE}{dt} = 0 \tag{5}$$

which means that the total mass M and the total energy E are conserved in the course of the time evolution.

(ii)

$$\frac{dH}{dt} \geq 0 \tag{6}$$

which means that the eta-function H can only grow during the time evolution.

(iii)

$$x \to x_{eq} \quad \text{as } t \to \infty \tag{7}$$

where x_{eq} is the state at which the thermodynamic potential

$$\Phi(x; T_{eq}, \mu_{eq}) = -H(x) + \frac{1}{T_{eq}} E(x) - \frac{\mu_{eq}}{M_{mol} T_{eq}} M(x), \tag{8}$$

reaches its minimum, i.e. a solution of

$$\Phi_x = 0. \tag{9}$$

The state x_{eq} is called an equilibrium state. The quantities M_{mol}, T_{eq} and μ_{eq} introduced in (8) are constant parameters. Their physical meaning is explained below.

2.6 Proofs

The property (5) follows from the skew-symmetry of L and from the degeneracy of L and Ξ.

By using the degeneracy of L, we arrive at $\frac{dH}{dt} = \langle H_x, \frac{\partial \Xi}{\partial H_x} \rangle \geq 0$. The last inequality follows from the properties required from the dissipation potential Ξ.

In order to prove the property (7) we note that the thermodynamic potential (8) plays the role of the Lyapunov function (i.e. Φ is convex and $\frac{d\Phi}{dt} \leq 0$). We have to stress however that this proof remains formal since the topological issues (needed already for proving that solutions to (1) exist) are not addressed.

2.7 The Fundamental Thermodynamic Relation of Classical Equilibrium Thermodynamics Implied by (1)

First, we introduced the state variables (E_{th}, N_{th}) of classical equilibrium thermodynamics: $E_{th} = E(x_{eq})$ is the equilibrium thermodynamic energy and $N_{th} = \frac{1}{M_{mol}} M(x_{eq})$ (M_{mol} is the molecular mass) is the equilibrium thermodynamic number of moles (both E_{th} and N_{th} per unit volume if the volume of the region in which the fluid under consideration is confined is put equal to one). Second, the conjugate form $P_{eq} = P_{eq}(\mu_{eq}, T_{eq})$ of the fundamental thermodynamic relation $S_{eq} = S_{eq}(E_{eq}, N_{eq})$ of classical equilibrium thermodynamics is the following:

$$-\frac{P_{eq}}{T_{eq}} = \Phi(x_{eq}; T_{eq}, \mu_{eq}) \tag{10}$$

P_{eq} is the equilibrium thermodynamic pressure, μ_{eq} the equilibrium thermodynamic chemical potential, T_{eq} the equilibrium thermodynamic temperature, and $S_{th} = H(x_{th})$ is the equilibrium thermodynamic entropy. The two forms $P_{eq} = P_{eq}(\mu_{eq}, T_{eq})$ and $S_{eq} = S_{eq}(E_{eq}, N_{eq})$ of the fundamental thermodynamic relation of classical equilibrium thermodynamic are related by the Legendre transformation.

3 GENERIC Constitutive Relations

The framework (1) is universal since it represents a mathematical expression of two universal experiences: compatibility with mechanics in the inviscid limit and the compatibility with thermodynamics in the case of externally unforced systems. The specific nature of the systems under investigation is expressed in the specification (called hereafter a GENERIC constitutive relations) of the state variables x, functions $E(x)$, $M(x)$, $H(x)$, $\Xi(H_x)$ and the operator $L(x)$, all introduced in (1). It is absolutely essential to make distinction between the universality of the framework and the non universality in the way it is filled. The framework (1) with x, E, M, H, Ξ, L specified is called a particular realization of (1). In the rest of this paper we shall make some general observations about various strategies that can be used to specify the GENERIC constitutive relations. We shall also work out an illustration.

3.1 State Variables

Before making general observations and developing the specific illustration, we present some examples of state variables x that have been explored.

In the first example (considered in [10]) we choose $x = (\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}), \boldsymbol{P}, \boldsymbol{Q})$. By ρ we denote the local mass (mass per unit volume), $\boldsymbol{u}$ is the momentum (momentum per unit volume), and e the energy (the total energy per unit volume); $\boldsymbol{r} \in \mathbb{R}^3$ denotes the position vector. By $(\boldsymbol{P}, \boldsymbol{Q})$ we denote the momenta and position vectors of $N \sim 10^3$ particles. This choice of state variables provides a setting for direct computer simulations (done with the main objective to obtain hydrodynamic fields as the result) of N particles that are subjected to external forces defined in terms of hydrodynamic fields (e.g. an imposed shear flow or a temperature control).

In the second example (considered in [11]) we take $x = (\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}), f(\boldsymbol{q}, \boldsymbol{p}))$, where $f(\boldsymbol{q}, \boldsymbol{p})$ is the one particle phase space distribution function, $\boldsymbol{q}$ is the momentum of one particle and $\boldsymbol{q}$ the position coordinate of one particle. The complete time evolution equations in this setting are in [11] ((40)–(43) in [11]). The one particle phase space distribution function represents in this setting an extra information about the system under consideration, i.e. an information in addition to the information provided by the classical hydrodynamic fields.

Grad's reformulation of kinetic theory in which the classical hydrodynamic fields arise as the first five moments (in the velocity variable) of the one particle phase space distribution function suggests [12, 13] to choose $x = (\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r})), \textit{higher order moments})$.

Investigations of complex fluids (e.g. polymeric fluids like the egg white or suspensions) lead [14–16] to the introduction of various extra fields characterizing either the internal structure of the suspended molecules and particles or their collective behavior. In both cases the extra field is typically a field $\psi(\boldsymbol{r}, \boldsymbol{R})$, where $\boldsymbol{R}$ is either the end-to-end vector of the suspended particle or the vector connecting two points in the suspension. In the latter case the field ψ is a pair correlation function.

Promotion of the classical hydrodynamic fields to the status of the random classical hydrodynamic fields represents another way [17–19] to introduce new x. We can also see the new state variables as $x = \mathcal{P}(\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}))$, where $\mathcal{P}$ denotes the distribution function.

By using the well established terminology, we refer to $x = (\textit{classical hydrodynamic fields})$ as macroscopic state variables, to $x = (\textit{classical hydrodynamic fields}, \textit{extra fields})$ or $x = (\textit{n-particle distribution functions})$, where $n = 1$ or $n = 2$ (rarely a larger integer) as mesoscopic state variables (a term coined by N.G. van Kampen), and to $x = (\boldsymbol{P}, \boldsymbol{Q})$ or $x = f_N(\boldsymbol{P}, \boldsymbol{Q})$, where $\boldsymbol{P}$ are momenta and $\boldsymbol{Q}$ position coordinates of $N \sim \textit{Avogadro's number}$ particles, $f_N(\boldsymbol{P}, \boldsymbol{Q})$ is the N-particle distribution function, as microscopic variables.

Now we turn to the question we want to address in this subsection: Given a physical system, the conditions in which it is observed, and our anticipated applications of the theory, what are the mesoscopic state variables x that we choose? The answer is based on a combination of the following three types of considerations.

(1) *Microscopic considerations.*

We choose a microscopic level (we denote it by the symbol $\mathcal{L}_{micro}$) and formulate on it the time evolution. The level $\mathcal{L}_{micro}$ can be the level of classical mechanics of $N \sim$ *Avogadro's number* of particles but it can also be, say, the level of one particle kinetic theory. Subsequently, we reduce the dynamics on the level $\mathcal{L}_{micro}$ to dynamics taking place on the level on which x serves as state variables. The reduction process is made in two steps. In the first step we solve completely the governing equations on the level $\mathcal{L}_{micro}$. As a result we obtain a collection of trajectories that we shall call a phase portrait on the level $\mathcal{L}_{micro}$; we shall denote it by the symbol $\mathcal{P}_{micro}$. In the second step we extract a pattern in $\mathcal{P}_{micro}$. The time evolution of the pattern is then the reduced dynamical theory that uses x as state variables. In general, new phenomena, new physics, emerge in the second step. In order to bring the second step closer to our everyday experience, we can think of $\mathcal{P}_{micro}$ as about a painting and about the pattern as about an emerging feature (e.g. human face). The two step reduction process sketched above is sometimes referred to as “an identification of slow variables and the slow time evolution”. It is obvious that the first step is prohibitively difficult (for example due to the enormous number of degrees of freedom and the lack of the complete microscopic characterization of the system under consideration). The second step is however even more difficult. Let us assume that we have succeeded to make the first step by analytically solving the governing equations on the level $\mathcal{L}_{micro}$. We are still very far from recognizing a pertinent pattern in $\mathcal{P}_{micro}$.

(2) *A guess based on an experience.*

Many macroscopic and mesoscopic theories (e.g. classical hydrodynamics) have been introduced (in a complete isolation from any microscopic point of view) in an attempt to organize and understand an experience collected in certain type of experimental observations. A large experience collected with complex fluids [12–16], in both experimental and theoretical investigations, can serve as a basis for suggesting a set of appropriate mesoscopic state variables x.

(3) *Anticipated applications.*

The choice of the state variables x is clearly influenced not only by the physics of the system under consideration but also by the anticipated applications. We shall naturally choose x that is as close as possible to what we directly observe and are interested in.

To sum up the above observations about an appropriate choice of x, we conclude that there is no completely satisfactory answer to the question “why this x, why not another”. The best we can do is to suggest x on the basis of a combination of the above three considerations. With such x we then calculate theoretical predictions and compare them with results of experimental observations. We can either be (relatively) satisfied or we are not satisfied and suggest another x.

3.1.1 Illustration

Below, we illustrate the process of constructing a particular realization of (1). As physical systems we choose simple fluids (e.g. water) in vicinity of the gas-liquid phase transition. Such fluids are expected to have three new features that in fact turn the simple fluid into a complex fluid: appearance of large spatial inhomogeneities, appearance of large fluctuations, and possibly also appearance of long range forces. The first and the third features will be addressed in the fundamental thermodynamic relation discussed in Sect. 3.2, the second and the third features are addressed below in the specification of extra fields admitted to x.

First, we begin with the anticipated applications of our mesoscopic theory. The fluids are expected to be observed with essentially the same experimental techniques as those used in classical hydrodynamics and in the experimental rheology of complex fluids. Our goal is to arrive at extended hydrodynamic equations of the type appearing in [20] (see also the references cited therein) and [21–23].

Second, we shall not turn to the microscopic analysis. We shall also avoid the stochastic approach in which $x = \mathcal{P}(\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}))$, where $\mathcal{P}$ denotes the distribution function. Our arguments proceed as follows.

The appearance of fluctuations is an indication that the quantities used as state variables (i.e. the classical hydrodynamic fields in our case) are insufficient. The fluctuations are caused by keeping out of control some other quantities playing an important role in the time evolution. What are these quantities? With the support from the vast experience collected in complex fluids we suggest that the pair correlation function $g(\boldsymbol{r}, \boldsymbol{R})$, where $\boldsymbol{R}$ is the vector connecting two points is one such quantity. With this new field we will also be able to express (in the specification of the fundamental thermodynamic relation discussed in Sect. 3.2 below) the influence long range forces that cannot be included into the setting of classical hydrodynamics. The choice of $g(\boldsymbol{r}, \boldsymbol{R})$ as the extra state variable can also be supported by the experience collected in equilibrium statistical mechanics [24]. Of course, the importance of the pair correlation function g recognized at equilibrium does not automatically mean that g retains its importance also in the time evolution. But here we argue that in the context of complex fluids (like suspensions) the pair correlations functions have been found (by comparing theoretical predictions with results of experimental observations) to be an appropriate state variables also out of equilibrium. Because of the relation between g and the extra stress tensor established in (33), we can also regard the acceptance of g into the set of state variables as an alternative way of accepting the stress tensor into x.

In the second field that we shall adopt into x we want to express genuine nonequilibrium processes. Candidates for such fields are the fluxes arising in the local conservation laws of classical hydrodynamic fields. This is indeed the way the extra fields are chosen in extended irreversible thermodynamics [12, 13]. We choose a field, we shall denote it $\boldsymbol{w}(\boldsymbol{r})$, that, as it will become clear later (in Sect. 4) when its role in the time evolution is revealed, is closely related to the nondissipative heat flux and entropy flux. We shall call $\boldsymbol{w}(\boldsymbol{r})$ an entropy-momentum since it will be shown to play the same role for the field of local entropy as the momentum $\boldsymbol{u}$ plays for the field of the local mass. Its relation to the heat flux is given in (43) and the entropy flux in (44) (see also Sect. 5.1.4 where the relation between $\boldsymbol{w}$ and the Fourier heat flux is established). Alternative arguments, different from those used in the extended irreversible thermodynamics [12, 13], that support the choice of $\boldsymbol{w}$ and provide it with an alternative physical interpretation have been introduced in [25, 26].

A general comment about the physical interpretation of the state variables x that are used in the context of the framework (1) is in order. It is well known in both mechanics and thermodynamics (both being present in (1)) that the state variables have always their conjugates (duals) and that it is very important to make a distinction between the variable and its dual. In thermodynamics, an example of such pair is the energy and the temperature. In mechanics, an example is the velocity and its dual called momentum. In the Hamiltonian formulation of mechanics, it is the momentum that presents itself as a natural state variable. Its dual, velocity, appears in the time evolution equations. Since the quantities that enter the time evolution equations are more directly related to the measured quantities, we can argue that the velocity is a more "physical" state variable than momentum. Nevertheless, it is with the momentum that we appreciate the mathematical structure of the time evolution equations and recognize its importance. This is indeed the reason why we use the momentum field $\boldsymbol{u}(\boldsymbol{r})$ instead of the velocity field $\boldsymbol{v}(\boldsymbol{r})$ that is customarily used in classical hydrodynamics. Similarly, the heat flux is a more "physical" quantity than the field $\boldsymbol{w}(\boldsymbol{r})$. Nevertheless, we have to use $\boldsymbol{w}(\boldsymbol{r})$ as the state variable since we are filling the Hamiltonian like structure (1). The same type of argument leads us to prefer the pair correlation function as the state variable over the extra stress tensor.

The full set of the state variables considered in this illustration of the extended hydrodynamics is thus

$$x = (\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}), g(\boldsymbol{r}, \boldsymbol{R}), \boldsymbol{w}(\boldsymbol{r})) \tag{11}$$

Next we should turn into the physics taking place on the boundaries. This type of consideration leads, in general, to another set of (boundary) state variables and boundary conditions for (11). In this paper we shall consider the fluids without boundaries. The boundary conditions for (11), if needed, will be the periodic boundary conditions.

3.2 Fundamental Thermodynamic Relation

With the state variables (11), the total energy E is clearly given by

$$E = \int d\boldsymbol{r} e(\boldsymbol{r}) \tag{12}$$

since $e(\boldsymbol{r})$, that is one of the fields included in the state variables (11), is, from the physical point of view, the local energy.

The total mass M is clearly

$$M = \int d\boldsymbol{r} \rho(\boldsymbol{r}) \tag{13}$$

since $\rho(\boldsymbol{r})$, that is one of the fields included in the state variables, has the physical meaning of the local mass.

The total entropy S is given by

$$S = \int d\boldsymbol{r} s(\boldsymbol{r}) \tag{14}$$

where $s(\boldsymbol{r})$ is the local entropy (entropy per unit volume)

$$s(\boldsymbol{r}) = s(\rho, \boldsymbol{u}, e, g, \boldsymbol{w}; \boldsymbol{r}) \tag{15}$$

Note that s depends on $\boldsymbol{u}$. This is because e is the total energy per unit volume (i.e. it includes the kinetic energy). It is customary in classical hydrodynamics to use the internal energy (that does not involve $\boldsymbol{u}$) and not the total energy as one of the hydrodynamics fields. If e in (15) is replaced by the internal energy then, due to the requirement of the Galilei invariance of the fundamental thermodynamic relation, $\boldsymbol{u}$ in (15) disappears (but $\nabla \boldsymbol{u}$ can still be there). We use in this paper the total instead of the internal energy since the structure of the governing equations as well as the equations themselves become much simpler.

Before discussing some particular examples of the relation (15), we introduce an equivalent reformulation of the fundamental thermodynamic relation (i.e. the specification of E, M and S). By using Callen's terminology [27], the state variables x considered so far have been the state variables in the entropy representation. If we solve the thermodynamic relation (15) for $e(\boldsymbol{r})$, we obtain the thermodynamic relation $e = e(y)$ where y are the state variables in which the field $e(\boldsymbol{r})$ is replaced by the local entropy $s(\boldsymbol{r})$. To simplify the notation, we shall use the same symbol x for the state variables in both representations:

$$x = (\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), s(\boldsymbol{r}), g(\boldsymbol{r}, \boldsymbol{R}), \boldsymbol{w}(\boldsymbol{r})) \tag{16}$$

Instead of (15) we thus have now

$$e(\boldsymbol{r}) = e(\rho, \boldsymbol{u}, s, g, \boldsymbol{w}; \boldsymbol{r}) \tag{17}$$

that plays the role of (15) in the energy representation. The one-to-one relation between $e(\boldsymbol{r})$ and $s(\boldsymbol{r})$ is guaranteed by the positivity of the local temperature $(e_{[s(\boldsymbol{r})]})^{-1}$). We use hereafter the notation: $A_{[\phi(\boldsymbol{r})]} = \frac{\delta A}{\delta \phi(\boldsymbol{r})}$, where A is a function of a field $\phi(\boldsymbol{r})$, and δ/δ is the Volterra functional derivative. For the later use we recall the relations among the derivatives of S and E:

$$E_{[s]} = (S_{[e]})^{-1}; \qquad E_{[u_i]} = -S_{[u_i]}/S_{[e]}; \qquad E_{[\rho]} = -S_{[\rho]}/S_{[e]}; \qquad E_{[w_i]} = -S_{[w_i]}/S_{[e]} \tag{18}$$

Now we turn to particular examples of the relation (15) or (17). We begin with (11) in which only the classical hydrodynamic fields $(\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}))$ are kept. Classical fluid mechanics assumes local equilibrium and consequently

$$s(\boldsymbol{r}) = s(\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r})) \tag{19}$$

is pointwise the thermodynamic relation representing the fluid under consideration in classical equilibrium thermodynamics.

We continue with (11) consisting of only the classical hydrodynamic fields. If the fluids under investigation involve important spatial gradients then the function s in (15) is expected to be nonlocal. Cahn and Hilliard [28] have extended (19) by letting $s(\boldsymbol{r})$ to depend also on the spatial gradient (denoted hereafter by the symbol ∇) of ρ, i.e. (19) is replaced by

$$s(\boldsymbol{r}) = s(\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}), \nabla\rho(\boldsymbol{r})) \tag{20}$$

If the gradients are not large, then, as suggested by Cahn and Hilliard, the extended fundamental thermodynamic relation (20) can be just the relation (19) to which a term proportional to $(\nabla\rho(\boldsymbol{r}))^2$ has been added. The equilibrium sate x_{eq} calculated for (8) in which H (called S in the particular setting discussed in this paper) in (14) involves (20) is, in general, spatially inhomogeneous. From the physical point of view, the appearance of the spatial inhomogeneity in x_{eq} can be interpreted as an appearance of gas-liquid phase transition. Indeed, van Kampen [24] has identified (20) for which the thermodynamic equation of state (10) is the van der Waals equation of state.

The equilibrium statistical mechanics can also be used (see e.g. [12]) to suggest the form of (15) if x involves the classical hydrodynamic fields and the pair correlation function g:

$$s(\boldsymbol{r}) = s(\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}), g(\boldsymbol{r}, \boldsymbol{R})), \nabla\rho(\boldsymbol{r}), \nabla e(\boldsymbol{r}), \nabla g(\boldsymbol{r}, \boldsymbol{R})) \tag{21}$$

We have included in (21) $\nabla\rho$, ∇e, and ∇g since, even at equilibrium, all three fields ρ, e, and g become spatially inhomogeneous in two-phase fluids.

Now we turn to nonequilibrium situations and thus to the two velocity-type fields $\boldsymbol{u}$ and $\boldsymbol{w}$ included in (15). If the state variables were position and momenta of all atoms composing the fluid under consideration then the kinetic energy were the sum of kinetic energies of all the atoms. This is the microscopic kinetic energy. If only $\boldsymbol{u}$ serves as the state variable then the kinetic energy is given by $E_{kin} = \int d\boldsymbol{r}\frac{\boldsymbol{u}^2}{2\rho}$ (called a macroscopic kinetic energy) and the difference between this energy and the sum of kinetic energies of all the atoms is included in the internal energy. If both $\boldsymbol{u}$ and $\boldsymbol{w}$ are included in the set of state variables then $E_{kin} = \int d\boldsymbol{r}(\frac{\boldsymbol{u}^2}{2\rho} + \frac{\boldsymbol{w}^2}{2\rho})$. This is a mesoscopic kinetic energy. The second term is a contribution of the molecular-level motion associated with the heat transfer. This term is included in the internal energy if $\boldsymbol{w}$ is absent in the set of state variables. We note that the mesoscopic kinetic energy is different from zero even in the absence of the overall motion (i.e. when $\boldsymbol{u} = 0$ and $\boldsymbol{w} \neq 0$. At the equilibrium however both $\boldsymbol{u}$ and $\boldsymbol{w}$ equal zero (since the equilibrium state is a solution of (9)) and consequently the kinetic energy equals zero.

The presence of spatial inhomogeneities of the mass field ρ brings by itself still another contribution to the kinetic energy. This is because the changes in ρ are in dynamical situations always accompanied with the occurrence of the divergence of the velocity. We shall therefore involve in the relation (21) also $\operatorname{div}\boldsymbol{u}$. (hereafter we shall use the notation $\nu = \operatorname{div}\boldsymbol{u}$) and write it as

$$s(\boldsymbol{r}) = s(\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}), g(\boldsymbol{r}, \boldsymbol{R})), \nabla\rho(\boldsymbol{r}), \nabla e(\boldsymbol{r}), \nabla g(\boldsymbol{r}, \boldsymbol{R}), \nu(\boldsymbol{r})) \tag{22}$$

The kinetic energy E_{kin} takes the form

$$E_{kin} = \int d\boldsymbol{r}\left(\frac{\boldsymbol{u}^2}{2\rho} + \frac{\boldsymbol{w}^2}{2\rho} + \frac{l^2\nu^2}{2\rho}\right) \tag{23}$$

where l is the characteristic length of the mass inhomogeneity. The last term in (23) is the contribution to the kinetic energy associated with the fluid motion needed to create or destroy spatial inhomogeneities. At the equilibrium $\boldsymbol{u} \equiv 0$ and thus also $\nu = 0$ so that the third term in (23) equals zero. But outside the equilibrium it represent an important contribution to the kinetic energy. The Cahn-Hilliard modification of the energy, developed originally by Cahn and Hilliard in the context of the equilibrium theory, has to be accompanied with the modification (23) of the kinetic energy if it is used in the context of a nonequilibrium theory. To the best of our knowledge, this intrinsically consistent extension of the Cahn-Hilliard analysis from equilibrium to nonequilibrium is made for the first time in this paper. Its interesting consequences for the time evolution will be discussed in Sects. 4 and 5.

If our interests were turned to complex, in particular then to turbulent, flows the we would involve in (22) also the vorticity. However, since we have in mind the same type of applications as those discussed in [20–23], we keep only the divergence of $\boldsymbol{u}$ (since this is the quantity closely related to changes in the mass density arising in gas-liquid phase transitions) and leave out the vorticity that becomes important in turbulent flows.

Finally, we add a comment about the functional derivatives introduced in (18). In the case when the nonlocal dependence is manifested only by involving spatial gradients but keeping the local (pointwise) functional dependence (i.e. the nonlocal dependence introduced (20), (21), and (22), the functional derivatives become variational functional derivatives:

$$A_{[\phi(\boldsymbol{r})]} = A_{\phi(\boldsymbol{r})} - \partial_i A_{\partial_i\phi(\boldsymbol{r})} + \partial_i\partial_j A_{\partial_i\partial_j\phi(\boldsymbol{r})} - \dots, \tag{24}$$

where $A_{\phi(\boldsymbol{r})}$ is the nonvariational (local) functional derivative of A with respect to $\phi(\boldsymbol{r})$, similarly $\partial_i A_{\partial_i\phi(\boldsymbol{r})}$ is the nonvariational (local) functional derivative of A with respect to $\partial_i\phi(\boldsymbol{r}), \dots$. By ∂_i we denote $\frac{\partial}{\partial r_i}$.

3.3 Kinematics

The state variables (11) are not new. Their kinematics is well known and readily available.

In order to be able to deal easily with the required degeneracy of L (i.e. the requirement that $LS_x = LM_x = 0$) we first introduce L in the energy representation (see (16)). The Poisson bracket (or equivalently the Poisson bivector L, see (3)) expressing the kinematics of (16) is given by

$$\{A, B\} = \int d\boldsymbol{r}(A_{[\rho]},\ A_{[\boldsymbol{u}]},\ A_{[s]},\ A_{[g]},\ A_{[\boldsymbol{w}]})L^e \begin{pmatrix} B_{[\rho]} \\ B_{[\boldsymbol{u}]} \\ B_{[s]} \\ B_{[g]} \\ B_{[\boldsymbol{w}]} \end{pmatrix} \tag{25}$$

$$\begin{aligned} &= \int d\boldsymbol{r}\big[\rho\big(\partial_j(A_{[\rho]})B_{[u_j]} - \partial_j(B_{[\rho]})A_{[u_j]}\big) \\ &\quad + u_j\big(\partial_i(A_{[u_j]})B_{[u_i]} - \partial_i(B_{[u_j]})A_{[u_i]}\big) \\ &\quad + s\big(\partial_j(A_{[s]})B_{[u_j]} - \partial_j(B_{[s]})A_{[u_j]}\big) \\ &\quad + s\big(\partial_j(A_{[s]})B_{[w_j]} - \partial_j(B_{[s]})A_{[w_j]}\big) \\ &\quad + \int d\boldsymbol{R} g\big(\partial_j(A_{[g]})B_{[u_j]} - \partial_j(B_{[g]})A_{[u_j]}\big) \\ &\quad + \int d\boldsymbol{R} g R_j\bigg(\frac{\partial}{\partial R_k}\big(A_{[g]}\big)\partial_j(B_{[u_k]}) - \frac{\partial}{\partial R_k}\big(B_{[g]}\big)\partial_j(A_{[u_k]})\bigg) \\ &\quad + w_j\big(\partial_i(A_{[w_j]})B_{[u_i]} - \partial_i(B_{[w_j]})A_{[u_i]}\big) \\ &\quad + w_j\big(\partial_i(A_{[w_j]})B_{[w_i]} - \partial_i(B_{[w_j]})A_{[w_i]}\big) \\ &\quad + w_j\big(\partial_i(A_{[u_j]})B_{[w_i]} - \partial_i(B_{[u_j]})A_{[w_i]}\big)\big] \end{aligned} \tag{26}$$

where A and B are sufficiently regular real valued functions of x. The derivatives appearing in (25) and (26) are the variational derivatives. Because of the nonlocal nature of the fundamental thermodynamic relations introduced in the previous section, the fact that the Poisson bracket involves the variational derivatives is of particular importance.

The degeneracy requirement $LS_x = LM_x = 0$ or equivalently $\{A, S\} = \{A, M\} = 0$ for all A can be directly verified for the bracket (26).

Before discussing the physics expressed in (26), we note that once the bracket is known in one representation it is also known in the other. This is because a one-to-one transformation $x \leftrightarrow y$ applied to the state variables transforms the Poisson bracket formulated in x into another Poisson bracket formulated in y. Moreover, both bracket satisfy the same degeneracy conditions. In particular then, if we transform x specified in (11) into x specified in (16) then the Poisson bracket (26) transforms into another Poisson bracket expressing kinematics of (16) satisfying the required degeneracy. We shall not write the new bracket explicitly but we shall use it below in Sect. 4 when we write the governing equations in both the entropy and the energy representations.

Now we turn to the explanation of the physics expressed in (26). In the particular case when the momentum field $\boldsymbol{u}(\boldsymbol{r})$ remains the only state variable (i.e. $x = \boldsymbol{u}(\boldsymbol{r})$), the Poisson bracket (26) reduces to $\{A, B\} =$ the second line in (26). This Poisson bracket indeed expresses the kinematics of the continuum. The argument goes as follows [9, 29]: The motion of the continuum is a Lie group of transformations $\mathbb{R}^3 \to \mathbb{R}^3$. The momentum field $\boldsymbol{u}$ can be seen as an element of the dual of the Lie algebra corresponding to this Lie group. In general, the Lie group operation induces always in the dual of its Lie algebra a Poisson bracket. The bracket $\{A, B\} =$ the first line in (26) is such bracket for the Lie group of the transformations $\mathbb{R}^3 \to \mathbb{R}^3$.

The remaining lines in the bracket (26) express the passive advection [29] of ρ by the overall velocity $E_{[\boldsymbol{u}]}$ (the first line), and of g also by $E_{[\boldsymbol{u}]}$ (the fifth and the sixth line). The terms involving w and s are obtained by first writing the Poisson bracket consisting of the first two lines but with $\boldsymbol{u}$ replaced by $\boldsymbol{w}$ and ρ by s. From the physical point of view, this corresponds to regarding the two pairs $(\rho, \boldsymbol{u})$ and $(s, \boldsymbol{w})$ as representing (as far as the kinematics is concerned) two components. This viewpoint of entropy (or alternatively energy) kinematics has been used already in [19, 20]. In order to obtain the third, the fourth and the last three lines in (26), we make in addition the one-to-one transformation $\boldsymbol{u} \to \boldsymbol{u} + \boldsymbol{w};\ \boldsymbol{w} \to \boldsymbol{w}$. The fact that the bracket (26) is a Poisson bracket follows directly from its construction. Alternatively, it is possible to verify directly its antisymmetry (that is clearly visible) and the Jacobi identity (this requires a long calculation).

3.4 Dissipation

Continuing the specification of the GENERIC constitutive relations, we turn to the dissipation potential Ξ. The attention on satisfying the degeneracy requirements of L lead us in the previous section to the energy representation. The same concern leads us in this section in the discussion of the dissipation potential Ξ to the entropy representation. The state variables x are thus in this section given in (11).

The role of the dissipation is to bring fluids to thermodynamic equilibrium. While the choice of the nondissipative time evolution is strongly constrained by requiring the Hamiltonian structure, the choice of the dissipative part of the time evolution is constrained only by requiring that the total mass, momentum and energy remain conserved, and that the total entropy does not decrease. The nondissipative dynamics is clearly more fundamental. We can see it by taking the fully microscopic (molecular) viewpoint of fluids. On this level the dynamics is only nondissipative. The dissipative part is absent. It will arises only in the process of solving the governing equations and interpreting the solutions (i.e. in the process of generating trajectories and searching in them a pattern pertinent to what is observed in macroscopic measurements). The extension that we are pursuing in this paper carries classical hydrodynamics to a level involving more details (nonlocalities and fluctuations). We expect therefore that the dissipation in the extended theory will be the same as, or weaker than, the dissipation in the classical theory.

We make therefore the following assumption: We keep the Navier-Stokes-Fourier dissipation of classical hydrodynamics [1–7] and add only the standard dissipation [15, 16] of the pair correlation and another standard dissipation [1, 2] of the field $\boldsymbol{w}$. We let the dissipation potential Ξ to depend on the following thermodynamic forces:

$$
\begin{aligned}
X_{ij}^{(u)} &= \frac{1}{2}(\partial_i (S_{[u_j]}/S_{[e]}) + \partial_j (S_{[u_i]}/S_{[e]})) \\
X^{(vol)} &= \partial_j (S_{[u_j]}/S_{[e]}) \\
X_i^{(w)} &= S_{w_i} \\
X_i^{(g)} &= \frac{\partial}{\partial R_i}(S_{[g]})
\end{aligned}
\tag{27}
$$

The thermodynamic potential itself is then given by

$$\Xi = \int d\boldsymbol{r} \frac{1}{2}\left[\eta X_{ij}^{(u)} X_{ij}^{(u)} + \left(\eta_{vol} - \frac{1}{3}\eta\right)(X^{(vol)})^2 + \lambda X_i^{(w)} X_i^{(w)} + \int d\boldsymbol{R} g \Lambda X_j^{(g)} X_j^{(g)}\right] \quad (28)$$

The first two terms represent the classical Navier-Stokes dissipation potential, η is the viscosity coefficient, η_{vol} is the volume viscosity coefficient. The third term is the term driving the field $\boldsymbol{w}$ to zero. We shall see this, as well as the relation of the phenomenological parameter λ, to the Fourier coefficient of heat conductivity, in Sect. 5.1.3. The fourth term is the standard dissipation potential in which the dissipation of the pair correlation function g is expressed. The coefficient Λ is a new phenomenological coefficient.

The properties required in Sect. 2 from Ξ (including its degeneracy) hold for (28) provided $\eta > 0$; $(\eta_{vol} - \frac{1}{3}\eta) > 0$; $\lambda > 0$; $\Lambda > 0$. This statement is proved easily by a direct verification.

4 Extended Hydrodynamic Equations

We have now all what we need to write explicitly the GENERIC equation (1). In this section we just make the calculations and report the result. There is nothing new (neither physics nor mathematics) entering this section. All the physics has been introduced in the concept of GENERIC (i.e. in (1)) and in the GENERIC constitutive relations. We shall return to physics in Sect. 5 where we shall interpret the governing equations and compare them with the equations arising in other extensions.

We begin with the Hamiltonian part in the energy representation, then we shall turn to the dissipative part in the entropy representation and finally to the complete hydrodynamic equations in the entropy representation.

By inserting (26) into

$$\left(\frac{\partial}{\partial t}\right)_{nondissip} \begin{pmatrix} \rho \\ \boldsymbol{u} \\ s \\ g \\ \boldsymbol{w} \end{pmatrix} = L^e \begin{pmatrix} E_{[\rho]} \\ E_{[\boldsymbol{u}]} \\ E_{[s]} \\ E_{[g]} \\ E_{[\boldsymbol{w}]} \end{pmatrix} \quad (29)$$

where L^e denotes the Poisson operator in the energy representation, we obtain the extended nondissipative time evolution equations

$$\begin{aligned}
\left(\frac{\partial \rho}{\partial t}\right)_{nondissip} &= -\partial_j(\rho E_{[u_j]}) \\
\left(\frac{\partial u_i}{\partial t}\right)_{nondissip} &= -\partial_j(u_i E_{[u_j]}) - \partial_i p - \partial_j \tau_{ij}^{(nd)} \\
\left(\frac{\partial s}{\partial t}\right)_{nondissip} &= -\partial_j(s E_{[u_j]}) - \partial_j(s E_{[w_j]}) \\
\left(\frac{\partial g}{\partial t}\right)_{nondissip} &= -\partial_j(g E_{[u_j]}) - \frac{\partial}{\partial R_i}(g R_j \partial_j E_{[u_i]}) \\
\left(\frac{\partial w_i}{\partial t}\right)_{nondissip} &= -\partial_j(w_i E_{[u_j]}) - \partial_j(w_i E_{[w_j]}) \\
&\quad - s\partial_i(E_{[s]}) - w_j \partial_i(E_{[u_j]}) - w_j \partial_i(E_{[w_j]})
\end{aligned} \quad (30)$$

where

$$p(\boldsymbol{r}) = -e(\boldsymbol{r}) + \rho(\boldsymbol{r})E_{[\rho(r)]} + s(\boldsymbol{r})E_{[s(r)]} + u_j(\boldsymbol{r})E_{[u_j(\boldsymbol{r})]} \\ + \int d\boldsymbol{R}g(\boldsymbol{r},\boldsymbol{R})E_{[g(r,R)]} + w_j E_{[w_j(\boldsymbol{r})]} \tag{31}$$

is the scalar hydrostatic pressure and

$$\tau_{ij}^{(nd)}(\boldsymbol{r}) = \tau_{ij}^{(g,w)}(\boldsymbol{r}) + \tau_{ij}^{(inhom)}(\boldsymbol{r}) \tag{32}$$

$$\tau_{ij}^{(g,w)}(\boldsymbol{r}) = -\int d\boldsymbol{R}g(\boldsymbol{r},\boldsymbol{R})R_j\frac{\partial}{\partial R_i}E_{g(r,R)} + w_i E_{w_j} \tag{33}$$

$$\tau_{ij}^{(inhom)}(\boldsymbol{r}) = \partial_i(\rho(\boldsymbol{r}))E_{\partial_j\rho(r)} + \partial_i(s(\boldsymbol{r}))E_{\partial_j s(r)} \\ + \frac{1}{2}E_{\nu(r)}(\partial_i(u_j(\boldsymbol{r})) + \partial_j(u_i(\boldsymbol{r}))) \\ + \int d\boldsymbol{R}\left(\partial_i(g(\boldsymbol{r},\boldsymbol{R}))E_{\partial_j g(r,R)} + g(\boldsymbol{r},\boldsymbol{R})R_j\frac{\partial}{\partial R_i}\partial_k E_{\partial_k g(r,R)}\right) \tag{34}$$

the elastic extra stress tensor.

The calculations involved in the passage from (26), (29) to (30)–(32) are completely straightforward. We just recall two useful identities:

$$\rho\partial_i\partial_j E_{\partial_j\rho} + \int d\boldsymbol{R}g\partial_i\partial_j E_{\partial_j g} + u_j\partial_i\partial_j E_\nu \\ -\rho\partial_i E_\rho - s\partial_i E_s - u_j\partial_i E_{u_j} - \int d\boldsymbol{R}g\partial_i E_g \\ = \partial_i\left(e - \rho E_\rho - sE_s - u_jE_{u_j} - gE_g + \rho\partial_j E_{\partial_j\rho} + u_j\partial_j E_\nu + \int d\boldsymbol{R}g\partial_j E_{\partial_j g}\right) \\ -\partial_j\left(\partial_i(\rho)E_{\partial_j\rho} + \partial_i(u_j)E_\nu + \int d\boldsymbol{R}\partial_i(g)E_{\partial_j g}\right) \tag{35}$$

and

$$-E_g\frac{\partial}{\partial R_i}(gR_j\partial_j(E_{u_i})) + E_{u_i}\partial_j\left(gR_j\frac{\partial}{\partial R_i}(E_g)\right) \\ = \partial_j\left(gR_j\frac{\partial}{\partial R_i}(E_g)E_{u_i}\right) - \frac{\partial}{\partial R_i}(gR_jE_g\partial_jE_{u_i}) \tag{36}$$

The most efficient way to arrive from (26), (29) to (30)–(32) is to use the form (4) of (2). To illustrate the calculations involved, we derive the first equation in (30). The left hand side of (4) equals $\int d\boldsymbol{r}A_\rho\partial\rho/\partial t + \dots$, where $\dots$ represents the terms involving derivatives of A with respect to the state variables except the field ρ. The right hand side of (4) we write (we use, if necessary, the integration by parts and the boundary conditions that make to disappear all the integrals over the boundaries that arise in the calculations) as $\int d\boldsymbol{r}A_\rho[\bullet] + \dots$, where $\dots$ represent again the terms involving derivatives of A with respect to the state variables except the field ρ. Since (4) is required to hold for all A, we obtain $\partial\rho/\partial t = [\bullet]$, which, if

[•] is written explicitly, is the first equation in (30). The same strategy we then use to obtain the time evolution equations for the remaining fields.

Now we turn to the dissipation part in the entropy representation:

$$\left(\frac{\partial}{\partial t}\right)_{dissip}\begin{pmatrix}\rho\\ \boldsymbol{u}\\ e\\ g\\ \boldsymbol{w}\end{pmatrix}=\begin{pmatrix}\Xi_{[S_{[\rho]}]}\\ \Xi_{[S_{[\boldsymbol{u}]}]}\\ \Xi_{[S_{[e]}]}\\ \Xi_{[S_{[g]}]}\\ \Xi_{S_{\boldsymbol{w}}}\end{pmatrix}\tag{37}$$

which, if written explicitly, becomes

$$\begin{aligned}\left(\frac{\partial\rho}{\partial t}\right)_{dissip}&=0\\ \left(\frac{\partial u_i}{\partial t}\right)_{dissip}&=-\partial_j\tau_{ij}^{(NS)}\\ \left(\frac{\partial e}{\partial t}\right)_{dissip}&=-\partial_j\left(\tau_{ji}^{(NS)}E_{[u_i]}\right)\\ \left(\frac{\partial g}{\partial t}\right)_{dissip}&=-\frac{\partial}{\partial R_j}\left(g\Lambda\frac{\partial}{\partial R_j}S_{[g]}\right)\\ \left(\frac{\partial w_i}{\partial t}\right)_{dissip}&=\lambda S_{w_i}\end{aligned}\tag{38}$$

where

$$\begin{aligned}\tau_{ij}^{(NS)}&=\eta\frac{1}{2}\frac{1}{S_{[e]}}(\partial_i(S_{[u_j]}/S_{[e]})+\partial_j(S_{[u_i]}/S_{[e]}))\\ &\quad+\frac{1}{S_{[e]}}\left(\eta_{vol}-\frac{1}{3}\eta\right)\partial_k(S_{[u_k]}/S_{[e]})\delta_{ij}\end{aligned}\tag{39}$$

is the Navier-Stokes stress tensor.

Finally, we write down the complete GENERIC equation (1) in the entropy representation. After transforming the Poisson bracket (26) into the entropy representation (we use below the symbol L^s to denote the transformed Poisson operator), we obtain

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \boldsymbol{u}\\ e\\ g\\ \boldsymbol{w}\end{pmatrix}=L^s\begin{pmatrix}0\\ 0\\ 1\\ 0\\ 0\end{pmatrix}+\begin{pmatrix}\Xi_{[S_{[\rho]}]}\\ \Xi_{[S_{[\boldsymbol{u}]}]}\\ \Xi_{[S_{[e]}]}\\ \Xi_{[S_{[g]}]}\\ \Xi_{S_{\boldsymbol{w}}}\end{pmatrix}\tag{40}$$

where L^s denotes the Poisson operator in the entropy representation. Written explicitly, (40) becomes

$$\begin{aligned}\frac{\partial\rho}{\partial t}&=-\partial_j(\rho E_{[u_j]})\\ \frac{\partial u_i}{\partial t}&=-\partial_j(u_iE_{[u_j]})-\partial_i p-\partial_j\tau_{ij}^{(nd)}-\partial_j\tau_{ij}^{(NS)}\end{aligned}$$

$$\begin{aligned}
\frac{\partial e}{\partial t} &= -\partial_j(eE_{[u_j]} + pE_{[u_j]} + (\tau_{ji}^{(g,w)} + \tau_{ji}^{(NS)})E_{[u_i]} + q_i^{(e)}) \\
\frac{\partial g}{\partial t} &= -\partial_j(gE_{[u_j]}) - \frac{\partial}{\partial R_i}(gR_j\partial_j E_{[u_i]}) \\
&\quad - \frac{\partial}{\partial R_j}\left(g\Lambda\frac{\partial}{\partial R_j}S_{[g]}\right) \\
\frac{\partial w_i}{\partial t} &= -\partial_j(w_i E_{[u_j]}) - \partial_j(w_i E_{[w_j]} \\
&\quad - s\partial_i(E_{[s]}) - w_j\partial_i(E_{[u_j]}) - w_j\partial_i(E_{[w_j]}) \\
&\quad + \lambda S_{w_i}
\end{aligned} \tag{41}$$

together with

$$\frac{\partial s}{\partial t} = -\partial_j(sE_{[u_j]}) - \partial_j q_j^{(s)} + \sigma \tag{42}$$

where p is given in (31), $\boldsymbol{\tau}^{(nd)}$ is given in (32), $\boldsymbol{\tau}^{(g,w)}$ in (33), $\boldsymbol{\tau}^{(NS)}$ in (39),

$$q_i^{(e)} = sE_{[s]}E_{[w_i]} + w_j E_{[w_j]}E_{[w_i]} \tag{43}$$

is the heat flux,

$$q_i^{(s)} = sE_{u_i]} + sE_{[w_i]} \tag{44}$$

is the entropy flux, and

$$\sigma = 2S_{[e]}\Xi \geq 0 \tag{45}$$

is the entropy production. The derivatives of E appearing in (41) and in (42) are understood to be expressed, by using the relation (18), in terms of derivatives of S.

The physical interpretation of the governing equations is discussed in the next section.

5 Comparison with Classical Hydrodynamics and Classical and Extended Irreversible Thermodynamics

The governing equations of extended hydrodynamics (41) have been obtained in Sect. 4 as a particular realization of GENERIC (1). This immediately means that the conservation laws (5) and the dissipation law (6) hold since they hold for the abstract dynamical system (1). Moreover, the equations governing the time evolution of the classical hydrodynamic fields have the form of the local conservation laws. To proceed further with the investigation of solutions of (41) and their comparison with results of experimental observations we need: (a) to identify the parameters that still remain unspecified in (41) for the fluids investigated experimentally, (b) to specify boundary conditions, and (c) to prepare appropriately the equations for introducing them into computers (i.e. to discretize them). In this paper we shall not follow this route. Instead, we shall concentrate on the comparison of the GENERIC approach and the classical way of constructing hydrodynamic equations. In this section we shall follow the classical approach. We begin with the local conservation laws for $\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r})$ and then proceed to specify the fluxes introduced in them (the so called classical constitutive relations).

Before doing it, we note already at this point an interesting difference between the GENERIC and the classical approach. Roughly speaking, the two approaches proceed in the reverse order. While the fluxes of the mass momentum, energy, and entropy arise as a result at the end of the GENERIC construction (in Sect. 4), their specification is the point of departure in the classical construction.

The new physics expressed in the extended theory has entered the GENERIC approach only in the specification of the state variables (Sect. 3.1) and the fundamental thermodynamic relation (Sect. 3.2). The rest, i.e. the kinematics (Sect. 3.3) and dissipation (Sect. 3.4), remained essentially the same as in the classical theory (except for the straightforward extensions needed to accommodate the new fields g and $\boldsymbol{w}$). We can thus regard the resulting extended hydrodynamics presented in Sect. 4 as an answer to the following question: what happens when the state variables (11) and the fundamental thermodynamic relation (22) are put into the GENERIC framework (1)? On the other hand, the new physics involved in the extension enters the classical approach gradually in the specification of the fluxes. One of the main difficulties met on this path is to retain the intrinsic compatibility of all the fluxes. In the GENERIC approach the compatibility is guaranteed automatically in all stages of the construction.

5.1 Classical Constitutive Relations

We shall now compare (41) with equations arising in other investigations of extensions of classical hydrodynamics.

5.1.1 Mass Flux

In the classical setting in which the state variables are only the fields $(\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}))$ and the fundamental thermodynamic relation is local, the mass flux $\boldsymbol{J}^{\rho}$ is postulated to be the momentum field: $\boldsymbol{J}^{\rho} = \boldsymbol{u}(\boldsymbol{r})$. The physics behind this specification is the following: the local mass conservation $\partial\rho/\partial t = -\mathrm{div}\, \boldsymbol{J}^{\rho}$ is regarded as a continuity (Liouville) equation corresponding to the motion of a fluid particle governed by $d\boldsymbol{r}/dt = \boldsymbol{v}(\boldsymbol{r})$, where $\boldsymbol{v}(\boldsymbol{r})$ is the velocity field.

In the GENERIC approach used in the classical setting, the mass flux (see the first equation in (41)) appears to be $\boldsymbol{J}^{\rho} = \rho E_{\boldsymbol{u}(\boldsymbol{r})}$. If we consider the classical setting in which only the first term in the kinetic energy (23) is different from zero then indeed $\rho E_{\boldsymbol{u}(\boldsymbol{r})} = \boldsymbol{u}(\boldsymbol{r})$ and thus the classical and the GENERIC mass fluxes are identical.

We proceed now to the extended setting in which the state variables are still only the classical fields $(\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}))$ but the fundamental thermodynamic relation involves spatial gradients. The mass flux $\boldsymbol{J}^{\rho}$ that the GENERIC theory (with the kinetic energy given in (23)) predicts is $\boldsymbol{J}^{\rho} = E_{[\boldsymbol{u}(\boldsymbol{r})]} = \boldsymbol{u}(\boldsymbol{r}) - l^2\nabla\nu(\boldsymbol{r})$. A similar result has already appeared in [1]. The physical interpretation of the new term $l^2\nabla\nu(\boldsymbol{r})$ is the same as the physical interpretation of the third term in the kinetic energy (23). Variations of the mass in space have to be accompanied with the mass flow that is not taken into account in the overall mass flow $\boldsymbol{u}(\boldsymbol{r})$.

In the classical approach, the mass flux that is not just the momentum but a sum of the momentum and the so called recoverable mass flux has been introduced in [30].

5.1.2 Momentum Flux

In the classical setting (i.e. when $x = (\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}))$ and the local equilibrium is assumed), the momentum flux is given by $\boldsymbol{J}^{u}_{ij} = \frac{u_i u_j}{\rho} + p\delta_{ij} + \tau^{(NS)}_{ij}$, where $p(\boldsymbol{r})$ is the local pressure and $\boldsymbol{\tau}^{(NS)}$ the Navier-Stokes extra stress tensor (39). The first term represents the passive advection of the momentum, the second term the force (acting on a surface element) due to the local pressure, and the third term the remaining such force. If we reduce the second equation in (41), (31) and (32) to the classical setting we see again a complete agreement between the GENERIC and the classical hydrodynamics.

In the extended setting in which we have still $x = (\rho(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}), e(\boldsymbol{r}))$ but the fundamental thermodynamic relation is allowed to be nonlocal, the momentum flux remains to be still composed of the three terms but all of them are modified. The momentum is advected now by $E_{[\boldsymbol{u}]}$ which, in the case when E depends on $\nu = \operatorname{div} \boldsymbol{u}$, is not only the overall velocity. The scalar hydrostatic pressure p (see (31)) is not any more just a local pressure but a pressure in which the nonlocal dependence is taken into account. The third term is modified most profoundly. A nondissipative (elastic) contribution $\boldsymbol{\tau}^{(inhom)}$ to the stress tensor arises as a consequence of the presence of inhomogeneities (see (32)). The inhomogeneous simple fluid becomes thus a viscoelastic fluid. With the exception of the modification of the first term, the other two modifications have already appeared in most of the papers (see [20] and the references cited therein, [21–23]) in which the classical route of extension is followed.

The presence of g and $\boldsymbol{w}$ in the state variables brings about still new terms in both p (see (31)) and $\boldsymbol{\tau}$ (see (32)). The two new terms in $\boldsymbol{\tau}$ (i.e. the term $\boldsymbol{\tau}^{(g,w)}$) are both known from previous investigations. The term involving the pair correlation function is familiar from the investigation of suspensions of rigid spherical particles [15, 16] (g is in this case the pair correlation of the suspended particles), the second term from extended irreversible thermodynamics [12, 13] in which an additional effort is made to reach beyond the linear formulation.

5.1.3 The Time Evolution of the Pair Correlation Function g

In the context of suspensions of rigid spherical particles, the equation governing the time evolution of g is known as the Smoluchowski equation [15, 16] or as the configuration space kinetic equations in [14]. The GENERIC approach thus provides its alternative derivation and, most importantly, shows how it is integrated in an intrinsically consistent manner into the set of the remaining time evolution equations.

5.1.4 The Time Evolution of the Entropy Momentum w

The equation governing the time evolution of a quantity that is related to the heat flux has been investigated in the extended irreversible thermodynamics [12, 13]. This approach requires conservation laws and the compatibility with thermodynamics but not the compatibility with mechanics (i.e. the Hamiltonian structure). Moreover, the exploitation of the entropy inequality (except if the Liu method [31] allowing a gradual ascent to higher order polynomial dependence is used) is limited to linear equations. Consequently, the nondissipative (nonlinear) part of the time evolution of $\boldsymbol{w}$ (i.e. the first five terms on the right hand side of the fifth equation in (41)) does not appear in [13]. We also note that the GENERIC method leads us to the velocity type field $\boldsymbol{w}$ that is only indirectly related to the heat flux (43) and the entropy flux (44). In extended irreversible thermodynamics it is the heat flux itself that is adopted as an independent state variable.

As we have mentioned already in Sect. 3.3, the kinematics of the field $\boldsymbol{w}$ is based on the physical considerations developed previously in [25, 26].

Finally, we make an observation about the relation of the equation governing the time evolution of the field $\boldsymbol{w}$ and the Fourier constitutive relation for the heat flux. Let $\boldsymbol{w}$ evolve much faster than the rest of the state variables. As $t \to \infty$, the field $\boldsymbol{w} \to 0$. Let us limit ourselves to the stage in the time evolution where $\partial \boldsymbol{w}/\partial t$ as well as $\boldsymbol{w}$ itself are very small. If we keep in the fifth equation in (41) only the terms linear in $\boldsymbol{w}$ we obtain: $\lambda S_{w_i} = s\partial_i E_{[s]}$. By inserting this relation into (43) we have $q_i^{(e)} = -\lambda^{(F)}\partial_i E_{[s]}$, where $\lambda^{(F)} = \frac{(sE_{[s]})^2}{\lambda}$ is the Fourier heat conductivity coefficient.

5.1.5 *Entropy Flux*

In the extended hydrodynamic that we have introduced in this paper the entropy is not just a passively advected scalar field but a field with its own dynamics. This is manifested by the presence of the second term in the entropy flux (44). From the physical point of view, we let the microscopic motion involved in the changes of the entropy (or alternatively the internal energy) to present itself on the mesoscopic level in the field $\boldsymbol{w}$.

5.1.6 *Energy Flux*

The energy flux is a sum of three terms: (i) the advection of e by the velocity $E_{[\boldsymbol{u}]}$ (the first term on the right hand side of the third equation in (41)), (ii) the work done during the flow (the second and the third terms on the right hand side of the third equation in (41), (iii) the heat flux (the fourth term on the right hand side of the third equation in (41). We note that the heat flux is irreversible (i.e. it changes its sign if the sign of ww and $\boldsymbol{u}$ is changed). We also note that the part $\boldsymbol{\tau}^{(inhom)}$ (see (34)) of the elastic extra stress tensor (i.e. the part that arises due to the spatial inhomogeneities) does not participate in the work done during the flow. The inhomogeneities enter the work only in the term involving the scalar hydrodynamic pressure p (see (31)).

Finally, we note that in the hydrodynamics in which the compatibility with thermodynamics is required, the time evolution of the energy and the entropy are closely interconnected. Important consequences of this physical feature for the mathematical properties of the governing equations (in particular for the implication that Cauchy's initial value problem is well posed) has been first realized in [32].

6 Concluding Remarks

We have introduced a new way to construct extensions of classical hydrodynamics. Both the new and the standard method can be seen as a search for particular realizations of an abstract dynamical system. In the standard method the abstract framework consists of the local conservation (balance) equations for the fields of the local mass, momentum and energy, in the new method it is GENERIC (1). The new feature that is incorporated into GENERIC is an appropriate (abstract) mathematical expression of the compatibility with classical mechanics.

The search for a new realization (called constitutive relations in the standard method and GENERIC constitutive relations in the GENERIC method) is an attempt to express the particular physics of the particular fluid under consideration in the quantities involved in the abstract dynamical system. It turns out, as it can be seen in the illustration worked out in this paper, that the starting point of the classical approach (i.e. specification of the fluxes in the local conservation laws) is the final point of the GENERIC approach.

The two methods should not be seen as one competing with the other but as being complementary. They offer two different paths to express a physical insight about a particular fluid in the governing equations of extended hydrodynamics.

The particular fluid discussed in this paper is a simple fluid in the vicinity of gas-liquid phase transition. The physics that we want to express and its consequence investigate is the presence of large spatial inhomogeneities and large fluctuations of classical hydrodynamic fields. We express the former by extending the fundamental thermodynamic relation from local to nonlocal and the latter by adopting two new fields into the set of state variables. One is the pair correlation function and the other is the field related to the heat flux. The most important new feature of the governing equations obtained by following the GENERIC extension is the guarantee of their intrinsic consistency. An appearance of a new term in one of the equations has to be accompanied with an appearance of appropriate new terms in the remaining equations. Specifically, we mention two interesting new results:

(i) The kinetic energy of the fluids involving large spatial inhomogeneities involves a term proportional to the square of the divergence of the velocity field. This term then brings about a modification of the way the hydrostatic pressure is expressed in terms of the state variables, and mainly, new advective fluxes. For example, the mass flux is no longer only the momentum but the momentum plus a term proportional to the gradient of the divergence of the velocity. This is the flux needed to create or destroy the spatial inhomogeneities.
(ii) The contribution (34) to the elastic extra stress tensor brought about by the local inhomogeneities does not participate in the energy balance.

An important advantage of the GENERIC approach is that it is directly applicable on any level of description. There is no restriction put on the choice of the state variable x. For example, we can choose x to be a one particular distribution function. The resulting realization of (1) would be then a kinetic equation. Still more interestingly, we can choose x to consist of the hydrodynamic fields and the one particle distribution function. With this choice the resulting realization would represent a multilevel (also called a multiscale) extension of classical hydrodynamics. We hope to explore the possibility of constructing multilevel models in a future paper.

Finally, we recall some previous investigation of the fluid discussed in this paper that were made on the level of kinetic theory. Let the state variable x be chosen to be the one point phase space distribution function $f(\boldsymbol{r}, \boldsymbol{v})$, where $\boldsymbol{r}$ and $\boldsymbol{v}$ is the position coordinate and the momentum of one particle (which can be a molecule or a "fluid particle"). If we make this choice of state variables, the next step is to introduce a kinetic equation governing the time evolution of $f(\boldsymbol{r}, \boldsymbol{v})$. In [33] such kinetic equation has been suggested on the basis of the following considerations. The essential physics entering the equilibrium van der Waals theory is the presence of two types of forces: the short range repulsive force and the long range attractive force. In the dynamical context of kinetic theory, the short range repulsive force finds its expression in the Enskog kinetic equation and the long range attractive force in the Vlasov equation. Their combination, termed in [25] the Enskog-Vlasov equation, is then a candidate for the kinetic equation of fluids undergoing gas-liquid phase transitions. The kinetic theory approach initiated in [33] has been then derived systematically and further investigated in [34–37].

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