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Korteweg-Type Fluids and Thermodynamic Modelling via Higher-Order Gradients

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Abstract: This paper investigates the modelling of Korteweg-type fluids and hence the dependence of the stress tensor on gradients of mass density. This topic, originating from the need for describing capillarity effects, is mainly of interest in connection with nanosystems where the mean free path may be comparable with the geometric dimensions of the system. In addition to the Korteweg fluid model, the paper gives a review of the stress tensor function arising in quantum fluid hydrodynamics. Next, thermodynamic consistency is established for a fluid involving first- and second-order density gradients. The modelling investigated is a generalization of the classical Korteweg fluid and allows a better understanding of previous thermodynamic restrictions. The restrictions determined for the general scheme with second-order gradients are applied to the particular cases of the Korteweg fluid and the quantum fluid. Further, to allow for discontinuity wave solutions with finite speed of propagation, a model is established which involves higher-order derivatives and reduces to the Korteweg fluid in stationary conditions.

Keywords: Korteweg fluids; quantum hydrodynamics; higher-order gradients; non-local equations; thermodynamic consistency; wave propagation

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1. Introduction

The modelling of fluids through higher-order spatial derivatives has received remarkable attention for several aspects. This attention is motivated by possible non-local properties of materials which are modelled by higher-order gradients. As an outstanding example, we mention that, to model the capillarity effects of liquids, Korteweg [1] proposed a constitutive equation for the stress tensor as a function of the first- and second-order gradients of the mass density. Likewise, in nanoscale systems, the mean free path may become comparable to the geometric dimensions and higher-order derivatives seem to be a reasonable way to set up a physically sound model [2]. As a comment, the (weak) non-locality through the use of higher-order derivatives is handier and more effective than that based on functionals on the whole region of the body.

Further, quantum models of diffusion are based on balance equations involving higher-order gradients of the mass density [3]. Lately, quantum hydrodynamics have been re-considered and investigated in a Korteweg-like form where the higher-order gradients of the mass density have a central role [4–6].

As is expected with models involving higher-order gradients, the system of equations pertaining to the Korteweg fluid or to quantum hydrodynamics are of parabolic character. This means that a disturbance at any point in the body is felt instantly at every other point or, otherwise, the speed of propagation of a disturbance is infinite. This feature can be checked by looking for the existence of discontinuity waves (see, e.g., [7], §175; [8], ch. 6). It seems natural that a physically sound model should be free from the paradox of infinite speed of propagation. To follow this idea, and meanwhile to keep the properties related to higher-order gradients, one might inspect the introduction of suitable higher-order time derivatives which, in stationary conditions, have no effect and yield the initial model.

The purpose of this paper is threefold. First, to review the pertinent equations and to show that both Korteweg-type fluids and quantum diffusion equations are framed within a common scheme of continuum mechanics. Secondly, to compute the possible restrictions placed by the compatibility with the second law of thermodynamics. The presence of higher-order gradients makes the continuum non-simple and requires that the thermodynamic analysis is developed within appropriate schemes, e.g., refs. [9,10] involve an undetermined entropy flux and ref. [11] allows for a vector field representing the interstitial working. Here, we investigate a general model involving density gradients not the particular Korteweg model. As an interesting particular case, the model of a Korteweg-type fluid is considered subject to flow incompressibility. Thirdly, to allow for discontinuity wave solutions with finite speed of propagation. This purpose is based on the observation that Korteweg-type models result in a third-order equation for mass density and that this equation is not compatible with discontinuity wave solutions. A model is established which involves higher-order derivatives and reduces to the Korteweg fluid in stationary conditions. The simplest method of generalization, that is considered in this paper, is to let the free energy depend on the time derivative of the mass density.

2. Notation and Balance Equations

We consider a fluid occupying a time-dependent region Ω in the three-dimensional space. The position vector of a point in Ω is denoted by $\mathbf{x}$. Hence, $\rho(\mathbf{x}, t)$ and $\mathbf{v}(\mathbf{x}, t)$ are the mass density and the velocity fields at $\mathbf{x}$, at time $t \in \mathbb{R}$. The symbol ∇ denotes the gradient, with respect to $\mathbf{x}$, while $\nabla\cdot$ is the divergence operator. For any pair of vectors $\mathbf{u}, \mathbf{w}$, or tensors $\mathbf{A}, \mathbf{B}$, the notations $\mathbf{u} \cdot \mathbf{w}$ and $\mathbf{A} \cdot \mathbf{B}$ denote the inner product. Cartesian coordinates are used and then, in the suffix notation, $\mathbf{u} \cdot \mathbf{w} = u_i w_i$, $\mathbf{A} \cdot \mathbf{B} = A_{ij} B_{ij}$, the summation over repeated indices being understood. Given a function g and a variable y, the symbol $\partial_y g$ denotes the partial derivative of g with respect to y. A superposed dot denotes the total time derivative and, hence, for any function $f(\mathbf{x}, t)$ on $\Omega \times \mathbb{R}$ we have $\dot{f} = \partial_t f + (\mathbf{v} \cdot \nabla) f$. The notation $a := b$ means a is defined to be equal to b. The symbol Δ denotes the Laplacian operator, 1 is the second-order identity tensor, and $\otimes$ denotes the dyadic product. Further, $\mathbf{T}$ is the Cauchy stress tensor, $\mathbf{D}$ the stretching, $\mathbf{W}$ the spin, ε the specific internal energy, $\mathbf{q}$ the heat flux vector, r the heat supply, θ the absolute temperature, and η the specific entropy. The symbols Sym and Skw denote the set of symmetric and skew-symmetric tensors. We let tr denote the trace and hence for any tensor, e.g., $\mathbf{D}$, we can write the decomposition, $\mathbf{D} = \mathbf{D}_0 + \frac{1}{3}(\mathrm{tr}\,\mathbf{D})1$, $\mathrm{tr}\,\mathbf{D}_0 = 0$.

The balance (conservation) of mass leads to the continuity equation in the form

$$\dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0 \qquad \text{or} \qquad \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0. \tag{1}$$

By the balance of linear momentum it follows

$$\rho \dot{\mathbf{v}} = \nabla \cdot \mathbf{T} + \rho \mathbf{b}. \tag{2}$$

It is standard to describe the viscosity effects via the Navier–Stokes model of the stress tensor $\mathbf{T}$. To account for capillarity effects, and hence for nonlocal properties, Korteweg [1] proposed the constitutive equation for $\mathbf{T}$ in the form

$$\mathbf{T} = (-p + \alpha_1 \Delta \rho + \alpha_2 |\nabla \rho|^2) 1 + \alpha_3 \nabla \rho \otimes \nabla \rho + \alpha_4 \nabla \nabla \rho + 2\mu \mathbf{D} + \lambda (\nabla \cdot \mathbf{v}) 1, \tag{3}$$

where $\alpha_1, ..., \alpha_4$, the pressure p, and the viscosity coefficients μ, λ are functions of ρ. In this case the system of differential Equations (1) and (2), along with appropriate initial and boundary conditions, can be investigated in the unknowns $\rho, \mathbf{v}$. If instead p and/or the coefficients α_i and μ, λ depend also on the temperature then a further equation (the balance of energy) is in order.

Irrespective of the form of the stress tensor, as, e.g., Equation (3), the balance of energy is taken in the standard form

$$\rho\dot{\varepsilon} = \mathbf{T}\cdot\mathbf{D} - \nabla\cdot\mathbf{q} + \rho r, \tag{4}$$

where ε is the energy density, $\mathbf{q}$ is the heat flux, and r is the heat supply.

Let θ be the absolute temperature and η the entropy density. Consistent with (2) and (4), we state the second law of thermodynamics by saying that the Clausius–Duhem inequality

$$\rho\dot{\eta} + \nabla\cdot\mathbf{j} - \frac{\rho r}{\theta} = \rho\gamma \geq 0 \tag{5}$$

has to hold for any thermodynamic process. Since the entropy flux $\mathbf{j}$ and the entropy production γ are given by constitutive equations [12] then the thermodynamic process consists of the functions $\rho, \mathbf{v}, \varepsilon, \mathbf{q}, r, \eta, \mathbf{j}, \gamma$ of $(\mathbf{x}, t) \in \Omega\times\mathbb{R}$.

For later convenience we point out that the equation of motion (2) is often written in a different form (see, e.g., [4]). Notice that

$$\rho\dot{\mathbf{v}} = \rho\partial_t\mathbf{v} + \rho(\mathbf{v}\cdot\nabla)\mathbf{v} = \partial_t(\rho\mathbf{v}) - \mathbf{v}\partial_t\rho + \nabla\cdot(\rho\mathbf{v}\otimes\mathbf{v}) - \mathbf{v}\nabla\cdot(\rho\mathbf{v}) = \partial_t(\rho\mathbf{v}) + \nabla\cdot(\rho\mathbf{v}\otimes\mathbf{v})$$

where Equation $(1)_2$ has been used. Hence, letting $\mathbf{J} = \rho\mathbf{v}$ we have the identity

$$\rho\dot{\mathbf{v}} = \partial_t\mathbf{J} + \nabla\cdot(\frac{\mathbf{J}\otimes\mathbf{J}}{\rho}).$$

Consequently, Equation (2) can be written in the form

$$\partial_t\mathbf{J} + \nabla\cdot(\frac{\mathbf{J}\otimes\mathbf{J}}{\rho}) = \nabla\cdot\mathbf{T} + \rho\mathbf{b}. \tag{6}$$

Two remarks are in order. First, Korteweg's starting point was an assumption of the form

$$\mathbf{T} + p\mathbf{1} = \mathfrak{F}(\mathbf{L}, \nabla\theta, \nabla\rho, \nabla\nabla\rho),$$

where $p = \hat{p}(\rho, \theta)$. In view of objectivity, if $\mathbf{Q}$ is the time-dependent rotation tensor of a Euclidean transformation [12] then the stress function $\mathfrak{F}$ is subject to

$$\mathbf{Q}\mathfrak{F}(\mathbf{L}, \nabla\theta, \nabla\rho, \nabla\nabla\rho)\mathbf{Q}^T = \mathfrak{F}(\mathbf{Q}\mathbf{D}\mathbf{Q}^T, \mathbf{Q}\nabla\theta, \mathbf{Q}\nabla\rho, \mathbf{Q}\nabla\nabla\rho\mathbf{Q}^T).$$

The particular case $\mathbf{Q} = -\mathbf{1}$ shows that only even-order terms in $\nabla\theta$ and $\nabla\rho$ can occur. That is why linear terms in $\nabla\theta$ cannot appear. Yet, without giving any reason, Korteweg dropped $\nabla\theta$ from the set of variables.

Secondly, we observe that the statement associated with (5) is an assumption. Relative to other approaches (see, e.g., [13], ch. 1, and refs therein), we do not distinguish formally equilibrium and non-equilibrium variables. Moreover, we consider irreversible processes as those providing $\gamma > 0$.

3. The Quantum Hydrodynamic System

The analogue of (1)–(3) holds in quantum hydrodynamics. To determine this analogue, we follow a standard approach. Observe that, if a quantum particle moves in free space, the wavefunction ψ evolves in time according to the Schrödinger equation

$$i\hbar\partial_t\psi = \big(-\frac{\hbar^2}{2m}\Delta + U\big)\psi, \tag{7}$$

where m is the mass of the particle, Δ is the Laplacian operator, and U is the potential of an applied force field. Since the wavefunction ψ is complex-valued then we let

$$\rho = \psi\psi^*$$

thus ascribing to $\rho(\mathbf{x}, t)$ the probability density, per unit volume, of finding the quantum particle at the point $\mathbf{x}$ at time t. We then represent ψ in the polar form

$$\psi = \sqrt{\rho}\exp(iS/\hbar),$$

and hence $S/\hbar = \arg\psi$. Both ρ and S are functions of $\mathbf{x}, t$. Upon evaluation of $\partial_t\psi$ and $\Delta\psi$ and substitution in (7) we find

$$i\hbar\big[\tfrac{1}{2}\rho^{-1/2}\partial_t\rho + \frac{i}{\hbar}\rho^{1/2}\partial_t S\big] = -\frac{\hbar^2}{2m}\big[-\tfrac{1}{4}\rho^{-3/2}|\nabla\rho|^2 + \tfrac{1}{2}\rho^{-1/2}\Delta\rho$$
$$+\frac{i}{\hbar}\rho^{-1/2}\nabla\rho\cdot\nabla S - \frac{1}{\hbar^2}\rho^{1/2}|\nabla S|^2 + \frac{i}{\hbar}\rho^{1/2}\Delta S + \rho^{1/2}U\big] \tag{8}$$

Notice that

$$\rho^{-1/2}\nabla\rho\cdot\nabla S + \rho^{1/2}\Delta S = \nabla\cdot(\rho^{1/2}\nabla S).$$

The imaginary part of (8) yields

$$\partial_t\rho = -\nabla\cdot(\rho\mathbf{v}), \qquad \mathbf{v} := \frac{1}{m}\nabla S. \tag{9}$$

Hence, the continuity Equation (1) is obtained by letting $m\mathbf{v} = \nabla S$. The real part of (8) results in

$$\partial_t S = -\frac{1}{2m}|\nabla S|^2 + \frac{\hbar^2}{2m}\big[\tfrac{1}{2}\rho^{-1}\Delta\rho - \tfrac{1}{4}\rho^{-2}|\nabla\rho|^2\big] - U.$$

In light of the identity

$$\tfrac{1}{2}\rho^{-1}\Delta\rho - \tfrac{1}{4}\rho^{-2}|\nabla\rho|^2 = \rho^{-1/2}\Delta\rho^{1/2}$$

we have

$$\partial_t S + \frac{1}{2m}|\nabla S|^2 = \frac{\hbar^2}{2m}\rho^{-1/2}\Delta\rho^{1/2} - U. \tag{10}$$

Notice that

$$\nabla|\nabla S|^2 = 2(\nabla S\cdot\nabla)\nabla S.$$

Hence, applying the gradient operator to (10) and dividing by m we obtain

$$\partial_t\mathbf{v} + (\mathbf{v}\cdot\nabla)\mathbf{v} = -\frac{1}{m}[\nabla Q + \nabla U], \tag{11}$$

where

$$Q := -\frac{\hbar^2}{2m\rho^{1/2}}\Delta\rho^{1/2}.$$

Equation (11) can be viewed as the equation of motion per unit mass; the function Q is often referred to as the Bohm quantum potential [14]. Equations (9) and (11) are also referred to as Madelung equations [15].

We now look for the continuum analogue of (2),

$$\rho[\partial_t\mathbf{v} + (\mathbf{v}\cdot\nabla)\mathbf{v}] = \rho[-\frac{1}{m}\nabla Q - \frac{1}{m}\nabla U].$$

It is natural to identify $-\nabla U/m$ with the body force $\mathbf{b}$. We then look for a stress tensor $\mathbf{T}$ such that

$$\nabla\cdot\mathbf{T} = -\rho\nabla\frac{Q}{m}.$$

First, we notice that

$$\Delta\rho^{1/2} = \nabla\cdot\nabla\rho^{1/2} = \nabla\cdot(\tfrac{1}{2}\rho^{-1/2}\nabla\rho) = -\tfrac{1}{4}\rho^{-3/2}|\nabla\rho|^2 + \tfrac{1}{2}\rho^{-1/2}\Delta\rho$$

and hence

$$-\frac{1}{m}\nabla Q = \frac{\hbar^2}{m^2}(\frac{1}{2\rho}\Delta\rho - \frac{1}{4\rho^2}|\nabla\rho|^2).$$

Letting $K(\rho) = 1/2\rho$ we can write

$$-\frac{1}{m}\nabla Q = \frac{\hbar^2}{m^2}(K(\rho)\Delta\rho + \tfrac{1}{2}K'(\rho)|\nabla\rho|^2).$$

The Quantum Stress Tensor

If a nonzero pressure $p(\rho)$ is allowed to occur then we can generalize the quantum equation of motion in the form

$$\rho\dot{\mathbf{v}} = -\nabla p(\rho) + \nu^2\rho\nabla(f(\rho)\Delta\rho + \tfrac{1}{2}f'(\rho)|\nabla\rho|^2) + \rho\mathbf{b},$$

where $\mathbf{b} = -\nabla U/m$ and $\nu = \hbar/m$. Now we show that there is a symmetric tensor $\mathbf{K}$ such that the equation of motion reads

$$\rho\dot{\mathbf{v}} = -\nabla p(\rho) + \nu^2\nabla\cdot\mathbf{K} + \rho\mathbf{b}.$$

Indeed, for any function $f(\rho)$ a direct check allows us to find that

$$\rho\nabla(f(\rho)\Delta\rho + \tfrac{1}{2}f'(\rho)|\nabla\rho|^2) = \nabla\cdot\mathbf{K},$$

where

$$\mathbf{K} = [\rho f'|\nabla\rho|^2 + \rho f\Delta\rho + \tfrac{1}{2}f|\nabla\rho|^2 - \tfrac{1}{2}\rho f'|\nabla\rho|^2]\mathbf{1} - f\nabla\rho\otimes\nabla\rho. \tag{12}$$

By defining the drift velocity

$$\mathbf{V} = \sqrt{f/\rho}\,\nabla\rho,$$

the tensor $\nu^2\mathbf{K}$ can be given the form of the viscous stress tensor of Navier–Stokes fluids [5]. Here, we merely observe that $\nu^2\mathbf{K}$ is a Korteweg-like stress tensor where

$$\alpha_1 = \rho f, \quad \alpha_2 = \tfrac{1}{2}(f + \rho f'), \quad \alpha_3 = f, \quad \alpha_4 = 0,$$

and account for viscosity in the classical way (3). In the particular case

$$f(\rho) = \frac{1}{2\rho}$$

it follows $f + \rho f' = 0$. Hence, $\mathbf{K}$ simplifies to

$$\mathbf{K} = \rho f\Delta\rho\,\mathbf{1} - f\nabla\rho\otimes\nabla\rho.$$

The present outline of quantum hydrodynamics gives the minimal content associated with the Korteweg fluid. Quantum hydrodynamics is developed in [16,17] in connection with superfluidity, where the model is based on coupled hydrodynamic equations for the superfluid and the normal fluid component. Also, quantum hydrodynamics enters the Bose–Einstein condensate [18,19] as a state that is formed when a gas of bosons at very low densities is cooled to temperatures close to absolute zero.

4. Thermodynamic Restrictions

We now examine the thermodynamic restrictions placed by thermodynamics on Korteweg-like stress tensors. For the sake of generality, or for an alternative approach, we do not require from the beginning that $\mathbf{T}$ is just in the form (3) or (12).

Let $\mathbf{j} = \mathbf{q}/\theta + \mathbf{k}$ and hence $\mathbf{k}$ represents the extra-entropy flux. Thus the Clausius–Duhem inequality (5) can be written in the form

$$\rho\dot{\eta} + \frac{1}{\theta}(\nabla\cdot\mathbf{q} - \rho r) + \nabla\cdot\mathbf{k} - \frac{1}{\theta^2}\mathbf{q}\cdot\nabla\theta = \rho\gamma \geq 0.$$

Substitution of $\nabla\cdot\mathbf{q} - \rho r$ from (4) and use of the Helmholtz free energy $\psi = \varepsilon - \theta\eta$ result in

$$-\rho(\dot{\psi} + \eta\dot{\theta}) + \mathbf{T}\cdot\mathbf{D} + \theta\nabla\cdot\mathbf{k} - \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta = \rho\theta\gamma \geq 0. \tag{13}$$

Based on the interest in constitutive equations of the Korteweg type (3), we might assume $\tilde{\Gamma} = (\theta, \rho, \nabla\theta, \nabla\rho, \dot{\rho}, \nabla\nabla\rho, \mathbf{D})$ is the set of variables. Now, by the continuity equation and the decomposition of $\mathbf{D}$,

$$\dot{\rho} = -\rho\nabla\cdot\mathbf{v}, \qquad \mathbf{D} = \mathbf{D}_0 + \tfrac{1}{3}(\operatorname{tr}\mathbf{D})1, \qquad \operatorname{tr}\mathbf{D} = \nabla\cdot\mathbf{v}, \tag{14}$$

We avoid redundancies by letting $\rho, \dot{\rho}$ account also for the dependence on $\nabla\cdot\mathbf{v}$. Hence, we assume

$$\Gamma = (\theta, \rho, \nabla\theta, \nabla\rho, \dot{\rho}, \nabla\nabla\rho, \mathbf{D}_0)$$

is the set of variables, and let $\psi, \eta, \mathbf{T}, \mathbf{q}, \mathbf{k}$, and γ be (constitutive) functions of Γ.

As for the constitutive function for the stress $\mathbf{T}$, we might take $\mathbf{T}$ as given by the Korteweg-type stress (3) or the quantum stress tensor (12). Yet, it is more interesting to regard $\mathbf{T}$, as well as the other constitutive quantities, as functions of Γ functions and next to examine the results in connection with (3) and (12).

Decompose the stress $\mathbf{T}$ in the standard way,

$$\mathbf{T} = -p1 + \boldsymbol{\mathcal{T}},$$

where p is the thermodynamic pressure, derived via a thermodynamic restriction. Hence, we compute $\dot{\psi}$ and $\nabla\cdot\mathbf{k}$ and substitute in (13) to obtain

$$\begin{aligned}-\rho(\partial_\theta\psi + \eta)\dot{\theta} + \rho^2\partial_\rho\psi\nabla\cdot\mathbf{v} - \rho\partial_{\nabla\theta}\psi\cdot(\nabla\theta)^{\cdot} - \rho\partial_{\nabla\rho}\psi\cdot(\nabla\rho)^{\cdot} - \rho\partial_{\dot{\rho}}\psi\ddot{\rho} - \rho\partial_{\mathbf{D}_0}\psi\cdot\dot{\mathbf{D}}_0\\ -\partial_{\nabla\nabla\rho}\psi\cdot(\nabla\nabla\rho)^{\cdot} - p\nabla\cdot\mathbf{v} + \boldsymbol{\mathcal{T}}\cdot\mathbf{D} - \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta + \theta\nabla\cdot\mathbf{k} = \rho\theta\gamma,\end{aligned} \tag{15}$$

and recall that $\dot{\rho} = -\rho\nabla\cdot\mathbf{v}$. To derive some necessary conditions placed by (15), we recall the identity (see Appendix A)

$$(\nabla g)^{\cdot} = \nabla\dot{g} - \mathbf{L}^T\nabla g \tag{16}$$

for any differentiable function $g(\mathbf{x}, t)$. Moreover, since $\mathbf{L} = \mathbf{D} + \mathbf{W}$, it follows

$$(\nabla g)^{\cdot} = \nabla\dot{g} - \mathbf{D}\nabla g + \mathbf{W}\nabla g. \tag{17}$$

Further,

$$(\nabla\nabla g)^{\cdot} = \nabla\nabla\dot{g} - (\mathbf{L}^T\nabla)\otimes\nabla g - \nabla[\mathbf{L}^T\nabla g].$$

Hence, if $g = \rho$ using (1) we find

$$(\nabla\nabla\rho)^{\cdot} = -(\nabla\nabla\rho)\nabla\cdot\mathbf{v} - 2\nabla\rho\otimes\nabla(\nabla\cdot\mathbf{v}) + \rho\nabla\nabla(\nabla\cdot\mathbf{v}) - (\mathbf{L}^T\nabla)\otimes\nabla\rho - \nabla\otimes[\mathbf{L}^T\nabla\rho]. \tag{18}$$

If $g = \theta$ we have $(\nabla\theta)^{\cdot} = \nabla\dot{\theta} - \mathbf{L}^T\nabla\theta$. Hence, $-\rho\partial_{\nabla\theta}\psi \cdot \nabla\dot{\theta}$ is the unique term that depends (linearly) on $\nabla\dot{\theta}$. The arbitrariness of $\nabla\dot{\theta}$ implies that

$$\partial_{\nabla\theta}\psi = 0. \tag{19}$$

Further, the linearity and arbitrariness of $\dot{\theta}$ imply

$$\eta = -\partial_\theta\psi. \tag{20}$$

By (18), $(\nabla\nabla\rho)^{\cdot}$ contains the term $\rho\nabla\nabla(\nabla\cdot\mathbf{v})$ and this term occurs in (15) only through $(\nabla\nabla\rho)^{\cdot}$. The linearity and arbitrariness of $(\nabla\nabla\rho)^{\cdot}$ imply that

$$\partial_{\nabla\nabla\rho}\psi = 0. \tag{21}$$

Since

$$\ddot{\rho} = \rho(\nabla\cdot\mathbf{v})^2 - \rho(\nabla\cdot\mathbf{v})^{\cdot}$$

the linearity and arbitrariness of $(\nabla\cdot\mathbf{v})^{\cdot}$ imply that

$$\partial_{\dot{\rho}}\psi = 0. \tag{22}$$

Likewise, by the occurrence of $\partial_{\mathbf{D}_0}\psi \cdot \dot{\mathbf{D}}_0$ and the arbitrariness of $\dot{\mathbf{D}}_0$, we conclude that

$$\partial_{\mathbf{D}_0}\psi = 0. \tag{23}$$

Consequently,

$$\psi = \psi(\theta, \rho, \nabla\rho).$$

For isotropic continua, the dependence of ψ on $\nabla\rho$ is through $|\nabla\rho|$. For formal convenience, we consider

$$\xi = \tfrac{1}{2}|\nabla\rho|^2$$

and let

$$\psi = \tilde{\psi}(\theta, \rho, \xi). \tag{24}$$

Hence, we have

$$\partial_{\nabla\rho}\psi = \partial_\xi\tilde{\psi}\,\nabla\rho. \tag{25}$$

In view of the restrictions (19)–(23), we can consider the simplified form of (15) and divide throughout by θ to obtain

$$\frac{1}{\theta}(\rho^2\partial_\rho\psi - p)\nabla\cdot\mathbf{v} - \frac{\rho}{\theta}\partial_{\nabla\rho}\psi\cdot(\nabla\rho)^{\cdot} + \frac{1}{\theta}\boldsymbol{\mathcal{T}}\cdot\mathbf{D} - \frac{1}{\theta^2}\mathbf{q}\cdot\nabla\theta + \nabla\cdot\mathbf{k} = \rho\gamma. \tag{26}$$

As for the term in $(\nabla\rho)^{\cdot}$, we notice that

$$(\nabla\rho)^{\cdot} = \nabla\dot{\rho} - \mathbf{L}^T\nabla\rho$$

and

$$-\frac{\rho}{\theta}\partial_{\nabla\rho}\psi\cdot\nabla\dot{\rho} = -\nabla\cdot(\frac{\rho}{\theta}\partial_{\nabla\rho}\psi\dot{\rho}) + [\nabla\cdot(\frac{\rho}{\theta}\partial_{\nabla\rho}\psi)]\dot{\rho}.$$

Hence, (26) can be written in the form

$$\frac{1}{\theta}(\rho^2\delta_\rho\psi - p)\nabla\cdot\mathbf{v} + \frac{\rho}{\theta}(\nabla\rho\otimes\partial_{\nabla\rho}\psi)\cdot\mathbf{L} + \frac{1}{\theta}\boldsymbol{\mathcal{T}}\cdot\mathbf{D} - \frac{1}{\theta^2}\mathbf{q}\cdot\nabla\theta + \nabla\cdot(\mathbf{k} - \frac{\rho}{\theta}\dot{\rho}\partial_{\nabla\rho}\psi) = \rho\gamma, \tag{27}$$

where

$$\delta_\rho\psi = \partial_\rho\psi - \frac{\theta}{\rho}\nabla\cdot(\frac{\rho}{\theta}\partial_{\nabla\rho}\psi).$$

We then let

$$\mathbf{k} = \frac{\rho}{\theta}\dot{\rho}\partial_{\nabla\rho}\psi$$

and look for the validity of the remaining condition. Since $\mathbf{L} = \mathbf{D} + \mathbf{W}$, then we have

$$\frac{\rho}{\theta}(\nabla\rho \otimes \partial_{\nabla\rho}\psi) \cdot \mathbf{W} + \ldots \geq 0,$$

the dots denoting terms independent of $\mathbf{W}$. The arbitrariness of $\mathbf{W} \in \mathrm{Skw}$ implies that

$$\nabla\rho \otimes \partial_{\nabla\rho}\psi \in \mathrm{Sym}$$

and then

$$\partial_{\nabla\rho}\psi \propto \nabla\rho;$$

this condition holds identically for the function $\psi(\theta, \rho, \xi)$. Consequently, upon multiplication by θ, we can write the remaining part of (27) in the form

$$(\rho^2\delta_\rho\psi - p)\nabla \cdot \mathbf{v} + [\rho(\nabla\rho \otimes \partial_{\nabla\rho}\psi) + \boldsymbol{\mathcal{T}}] \cdot \mathbf{D} - \frac{1}{\theta}\mathbf{q} \cdot \nabla\theta = \rho\gamma, \tag{28}$$

Notice that, since (24) and (25), we compute $\delta_\rho\psi$ to find

$$\begin{aligned}\delta_\rho\psi &= \partial_\rho\tilde{\psi} - \tfrac{\theta}{\rho}\nabla \cdot (\tfrac{\rho}{\theta}\partial_\xi\tilde{\psi}\nabla\rho) \\ &= \partial_\rho\tilde{\psi} - \theta\partial_\theta(\tfrac{1}{\theta}\partial_\xi\tilde{\psi})\nabla\theta \cdot \nabla\rho - \tfrac{1}{\rho}\partial_\rho(\rho\partial_\xi\tilde{\psi})|\nabla\rho|^2 - \partial^2_\xi\tilde{\psi}\nabla\xi \cdot \nabla\rho - \partial_\xi\tilde{\psi}\Delta\rho\end{aligned} \tag{29}$$

while

$$\nabla\xi \cdot \nabla\rho = \nabla\rho \cdot (\nabla\rho \cdot \nabla)\nabla\rho = (\nabla\rho \otimes \nabla\rho) \cdot \nabla\nabla\rho. \tag{30}$$

For later purposes, we let

$$\delta_\rho\psi = \overline{\delta_\rho\psi} - \theta\partial_\theta(\frac{1}{\theta}\partial_\xi\tilde{\psi})\nabla\theta \cdot \nabla\rho,$$

thus defining $\overline{\delta_\rho\psi}$.

We notice also that

$$(\nabla\rho \otimes \partial_\xi\tilde{\psi}\nabla\rho) \cdot \mathbf{D} = \partial_\xi\tilde{\psi}(\nabla\rho \otimes \nabla\rho) \cdot \mathbf{D}_0 + \tfrac{1}{3}\partial_\xi\tilde{\psi}|\nabla\rho|^2\nabla \cdot \mathbf{v}.$$

Further consequences of (28) follow depending on appropriate assumptions about $\boldsymbol{\mathcal{T}}$ and $\mathbf{q}$.

(1) Assume $\boldsymbol{\mathcal{T}} = \boldsymbol{\mathcal{T}}^{\mathrm{el}} + \boldsymbol{\mathcal{T}}^{\mathrm{vis}}$, with $\boldsymbol{\mathcal{T}}^{\mathrm{vis}} \to 0$ as $\mathbf{D} \to 0$, and $\mathbf{q}$ is independent of the stretching $\mathbf{D}$.

The linearity and arbitrariness of $\mathbf{D}$ imply that

$$\boldsymbol{\mathcal{T}}^{\mathrm{el}} - p\mathbf{1} + \rho^2\delta_\rho\psi\,\mathbf{1} + \rho\partial_\xi\tilde{\psi}\nabla\rho \otimes \nabla\rho = 0.$$

Hence, we can obtain a non-negative entropy production by letting $\boldsymbol{\mathcal{T}}^{\mathrm{vis}}$ be the classical viscous stress so that

$$\mathbf{T} = \boldsymbol{\mathcal{T}} - p\mathbf{1} = -\rho^2\delta_\rho\psi\mathbf{1} + \rho\partial_\xi\tilde{\psi}\nabla\rho \otimes \nabla\rho + 2\mu\mathbf{D} + \lambda(\mathrm{tr}\,\mathbf{D})\mathbf{1}, \tag{31}$$

$$\mathbf{q} = -\kappa\nabla\theta,$$

where $\mu(\theta,\rho), \lambda(\theta,\rho), \kappa(\theta,\rho)$ are subject to the the standard relations $\mu \geq 0, \lambda + 2\mu/3 \geq 0$, $\kappa \geq 0$.

The decomposition of $\mathbf{T}$ in $\boldsymbol{\mathcal{T}}^{\mathrm{el}}$ and $-p\mathbf{1}$ is not unique unless we fix $\mathrm{tr}\,\boldsymbol{\mathcal{T}}$ or p. For definiteness, we might assume $p = p(\theta, \rho)$ and then

$$p = \rho^2\partial_\rho\Psi, \qquad \psi = \Psi(\theta, \rho) + \hat{\psi}(\theta, \xi).$$

Hence, using (29) and (30), we obtain from (31) that

$$\boldsymbol{\mathcal{T}} = [\rho^2\theta\partial_\theta(\frac{1}{\theta}\partial_\xi\hat{\psi})\nabla\theta\cdot\nabla\rho + \rho\partial_\rho(\rho\partial_\xi\hat{\psi})|\nabla\rho|^2 + \rho^2\partial^2_\xi\hat{\psi}(\nabla\rho\otimes\nabla\rho)\cdot\nabla\nabla\rho$$
$$+\rho^2\partial_\xi\hat{\psi}\Delta\rho]\mathbf{1} - \rho\partial_\xi\hat{\psi}\nabla\rho\otimes\nabla\rho + 2\mu\mathbf{D} + \lambda(\mathrm{tr}\,\mathbf{D})\mathbf{1}. \tag{32}$$

(2) The heat flux $\mathbf{q}$ is allowed to depend on $\nabla\cdot\mathbf{v}$ while $\boldsymbol{\mathcal{T}} = \boldsymbol{\mathcal{T}}^{\mathrm{el}} + \boldsymbol{\mathcal{T}}^{\mathrm{vis}}$, with $\boldsymbol{\mathcal{T}}^{\mathrm{vis}} \to 0$ as $\mathbf{D}\to 0$ and $\partial_{\nabla\theta}\boldsymbol{\mathcal{T}} = 0, \partial_{\nabla\theta}p = 0$.

Let $\nabla\theta = 0$. We then write (28) in the form

$$(\rho^2\overline{\delta_\rho\psi} - p)\nabla\cdot\mathbf{v} + [\rho\partial_\xi\psi\nabla\rho\otimes\nabla\rho + \boldsymbol{\mathcal{T}}]\cdot\mathbf{D} - [\rho^2\theta\partial_\theta(\frac{1}{\theta}\partial_\xi\psi)\nabla\cdot\mathbf{v}\,\nabla\rho + \frac{1}{\theta}\mathbf{q}]\cdot\nabla\theta = \rho\theta\gamma. \tag{33}$$

Let $\nabla\theta = 0$. If we let $p = \rho^2\partial_\rho\Psi$, by assumption then it follows from (33) that

$$\mathbf{T} = -\rho^2[\partial_\rho\Psi - \frac{1}{\rho}\partial_\rho(\rho\partial_\xi\hat{\psi})|\nabla\rho|^2 - \partial^2_\xi\hat{\psi}(\nabla\rho\otimes\nabla\rho)\cdot\nabla\nabla\rho - \partial_\xi\hat{\psi}\Delta\rho]\mathbf{1}$$
$$-\rho\partial_\xi\hat{\psi}\nabla\rho\otimes\nabla\rho + 2\mu\mathbf{D} + \lambda(\mathrm{tr}\,\mathbf{D})\mathbf{1}. \tag{34}$$

The remaining condition has to hold for arbitrary values of $\nabla\theta$ and this happens if

$$\mathbf{q} + \rho^2\theta^2\partial_\theta(\frac{1}{\theta}\partial_\xi\hat{\psi})\nabla\cdot\mathbf{v}\,\nabla\rho = -\kappa\nabla\theta;$$

if $\partial_\xi\hat{\psi} = \theta$ then the standard Fourier law follows.

As an aside, depending on the assumption on the heat flux $\mathbf{q}$ and the stress tensor $\mathbf{T}$, the entropy production

$$-\rho\partial_\theta(\frac{1}{\theta}\partial_\xi\hat{\psi})\nabla\theta\cdot\nabla\rho\nabla\cdot\mathbf{v}$$

is viewed as the effect of the partial pressure

$$-\rho^2\theta\partial_\theta(\frac{1}{\theta}\partial_\xi\hat{\psi})\nabla\theta\cdot\nabla\rho$$

or the effect of the partial heat flux

$$-\rho^2\theta^2\partial_\theta(\frac{1}{\theta}\partial_\xi\hat{\psi})\nabla\cdot\mathbf{v}\,\nabla\rho.$$

5. Relation to Korteweg-Type Stress Tensors

The constitutive functions (32) and (34) for the stress are derived within a thermodynamic setting where the free energy ψ and the stress $\mathbf{T}$ are considered from the start as functions of $(\theta,\rho,\dots)$. Instead, as it happens, e.g., in [10,11], we can investigate the thermodynamic consistency of the stress $\mathbf{T}$ directly in Korteweg form. It is then of interest to contrast the present results with those obtained directly with the constitutive function (3).

It is worth remarking the differences in the approaches of [10,11]. The analysis in [11] is developed by allowing for an extra-energy flux ascribed to interstitial working and no extra-entropy flux. Instead, ref. [10] allows for an extra-entropy flux and investigates the thermodynamic consistency by applying the Liu procedure [20] to a Korteweg-type stress function with the additional term $\alpha_5(\nabla\cdot\mathbf{v})\mathbf{1} + \alpha_6\mathbf{L}$. The occurrence of $\alpha_5(\nabla\cdot\mathbf{v})\mathbf{1}$ looks here inessential in that the stress involves the viscous term $\lambda(\nabla\cdot\mathbf{v})\mathbf{1}$. The occurrence of $\alpha_6\mathbf{L}$ is quite subtle in that objectivity would require that $\boldsymbol{\mathcal{T}}$ be independent of the spin $\mathbf{W}$.

Look at Equation (32) for the stress $\boldsymbol{\mathcal{T}}$. Observe that the $\nabla\theta\cdot\nabla\rho$ term in $\boldsymbol{\mathcal{T}}$ occurs simply because we allow ψ to depend jointly on $\nabla\rho$ (through ξ) and θ. This effect is avoided if we assume $\psi = \Psi(\theta,\rho) + \hat{\psi}(\xi)$. Hence, we omit writing the $\nabla\theta\cdot\nabla\rho$ term and the standard viscous terms $2\mu\mathbf{D} + \lambda(\mathrm{tr}\,\mathbf{D})1$. The constitutive Equation (32) is then simplified to

$$\boldsymbol{\mathcal{T}} = [\rho\partial_\rho(\rho\partial_\xi\hat{\psi})|\nabla\rho|^2 + \rho^2\partial^2_\xi\hat{\psi}(\nabla\rho\otimes\nabla\rho)\cdot\nabla\nabla\rho + \rho^2\partial_\xi\hat{\psi}\Delta\rho]1 - \rho\partial_\xi\hat{\psi}\nabla\rho\otimes\nabla\rho. \quad (35)$$

The analogous expressions of Korteweg stress tensor $\boldsymbol{\mathcal{T}}_K$ and the quantum stress tensor $\boldsymbol{\mathcal{T}}_Q = \nu^2\mathbf{K}$ are

$$\boldsymbol{\mathcal{T}}_K = (\alpha_1\Delta\rho + \alpha_2|\nabla\rho|^2)1 + \alpha_3\nabla\rho\otimes\nabla\rho + \alpha_4\nabla\nabla\rho, \quad (36)$$

$$\boldsymbol{\mathcal{T}}_Q = \nu^2\{[\rho f\Delta\rho + \tfrac{1}{2}(f+\rho f')|\nabla\rho|^2]1 - f\nabla\rho\otimes\nabla\rho\}. \quad (37)$$

Both [10,11] find that $\alpha_4 = 0$. This result is consistent with the expression (35) where the tensor $\nabla\nabla\rho$ does not occur. Instead, and consistent with [11], $\nabla\nabla\rho$ occurs through the scalar $(\nabla\rho\otimes\nabla\rho)\cdot\nabla\nabla\rho$, not, by definition, in the Korteweg stress (36).

The tensor $\nabla\rho\otimes\nabla\rho$ as such occurs consistently in the present derivation (35) and in the Korteweg stress (36).

Further, both $|\nabla\rho|^2$ and $\Delta\rho$ occur in (35) and (36).

Differences arise for the quantum stress tensor $\boldsymbol{\mathcal{T}}_Q$ relative to $\boldsymbol{\mathcal{T}}$ and $\boldsymbol{\mathcal{T}}_K$ in that it is free of $\nabla\nabla\rho$ in any form. Rather, $\boldsymbol{\mathcal{T}}_Q$ contains even $|\nabla\rho|^2$ and $\Delta\rho$ as it happens for $\boldsymbol{\mathcal{T}}$ and $\boldsymbol{\mathcal{T}}_K$. In summary, comparing (36) and (37) with (35), we have

$$\begin{aligned} \boldsymbol{\mathcal{T}}_K: &\quad \alpha_1 = \rho^2\partial_\xi\hat{\psi}, \quad \alpha_2 = \rho\partial_\rho(\rho\partial_\xi\hat{\psi}), \quad \alpha_3 = -\rho\partial_\xi\hat{\psi}, \quad \alpha_4 = 0, \\ \boldsymbol{\mathcal{T}}_Q: &\quad \nu^2\rho f = \rho^2\partial_\xi\hat{\psi}, \quad \tfrac{1}{2}\nu^2(f+\rho f') = \rho\partial_\rho(\rho\partial_\xi\hat{\psi}), \quad \nu^2 f = \rho\partial_\xi\hat{\psi}. \end{aligned} \quad (38)$$

Differences and analogies justify the view of the quantum stress tensor $\boldsymbol{\mathcal{T}}_Q$ as a Korteweg-like stress tensor. Yet the quantum stress $\boldsymbol{\mathcal{T}}_Q$ enjoys a peculiar property in that, if $f = 1/2\rho$, then

$$f + \rho f' = 0$$

and $\boldsymbol{\mathcal{T}}_Q$ simplifies to

$$\boldsymbol{\mathcal{T}}_Q = \nu^2[\rho f\Delta\rho\,1 - f\nabla\rho\otimes\nabla\rho].$$

We still need a formulation of the second law of thermodynamics for quantum systems within a continuum context. This suggests that we investigate the consistency of the correspondences (38) and hence look for a potential $\hat{\psi}$ of quantum systems. The first and the third correspondences yield $\nu^2 f = \rho\partial_\xi\hat{\psi}$. Substitution in the second correspondence results in

$$\rho f' = f$$

whence

$$f = c\rho, \qquad \hat{\psi} = \nu^2 c\rho,$$

c being a constant. This shows that the assumption $f + \rho f' = 0$ leads to a contradiction of the requirement (38).

6. Dynamic Properties of the Korteweg Fluid

The unknown triplet $(\rho, \mathbf{v}, \theta)$ of a dynamic problem is determined by the balance equations along with the constitutive equation for the stress $\mathbf{T}$. For definiteness, we consider the constitutive Equation (31) and, for simplicity, we let the fluid be inviscid so that $\mu = 0$ and $\lambda = 0$. Moreover, we let

$$\psi = \Psi(\theta,\rho) + \hat{\psi}(\xi).$$

Hence, we have

$$\varepsilon = \Psi(\theta,\rho) + \hat{\psi}(\xi) - \theta\partial_\theta\Psi(\theta,\rho) = \varepsilon(\theta,\rho,\nabla\rho).$$

and

$$\mathbf{T} = -\rho^2 \delta_\rho \psi 1 + \rho \partial_\xi \hat{\psi} \nabla \rho \otimes \nabla \rho$$

while

$$\delta_\rho \psi = \partial_\rho \Psi + \frac{1}{\theta} \partial_\xi \hat{\psi} \nabla \theta \cdot \nabla \rho - \frac{1}{\rho} \partial_\xi \hat{\psi} |\nabla \rho|^2 - \partial_\xi^2 \hat{\psi} (\nabla \rho \otimes \nabla \rho) \cdot \nabla \nabla \rho - \partial_\xi \hat{\psi} \Delta \rho.$$

Consequently,

$$\mathbf{T} = \mathbf{T}_1(\theta, \rho, \nabla \theta, \nabla \rho) + [\rho^2 \partial_\xi^2 \hat{\psi} (\nabla \rho \otimes \nabla \rho) \cdot \nabla \nabla \rho + \rho^2 \partial_\xi \hat{\psi} \Delta \rho] 1 + \rho \partial_\xi \hat{\psi} \nabla \rho \otimes \nabla \rho, \tag{39}$$

where

$$\mathbf{T}_1 = [-\rho^2 \partial_\rho \Psi - \frac{\rho^2}{\theta} \partial_\xi \hat{\psi} \nabla \theta \cdot \nabla \rho + \rho \partial_\xi \hat{\psi} |\nabla \rho|^2] 1.$$

It follows that

$$\nabla \cdot \mathbf{T} = \mathbf{f}(\theta, \rho, \nabla \theta, \nabla \rho, \nabla \nabla \theta, \nabla \nabla \rho) + \rho^2 [\partial_\xi^2 \hat{\psi} (\nabla \rho \otimes \nabla \rho) \nabla \nabla \nabla \rho + \partial_\xi \hat{\psi} \nabla \Delta \rho].$$

Hence, the dynamic equations can be written in the form

$$\dot{\rho} = -\rho \nabla \cdot \mathbf{v},$$

$$\rho \dot{\mathbf{v}} = \mathbf{f}(\theta, \rho, \nabla \theta, \nabla \rho, \nabla \nabla \theta, \nabla \nabla \rho) + \rho^2 [\partial_\xi^2 \hat{\psi} (\nabla \rho \otimes \nabla \rho) \nabla \nabla \nabla \rho + \partial_\xi \hat{\psi} \nabla \Delta \rho] + \rho \mathbf{b},$$

$$\begin{aligned} (\rho \dot{\varepsilon})(\theta, \rho, \nabla \rho, \dot{\theta}, \dot{\rho}, (\nabla \rho)^{\cdot}) &= \mathbf{T}(\theta, \rho, \nabla \theta, \nabla \rho, \nabla \nabla \rho) \cdot \mathbf{D} \\ &- (\nabla \cdot \mathbf{q})(\theta, \rho, \nabla \theta, \nabla \rho, \nabla \nabla \theta, \nabla \nabla \rho) + \rho r, \end{aligned}$$

where $\mathbf{b}$ and r are assumed to be known functions of $\mathbf{x}$ and t. The dynamic equations constitute a system of third-order differential equations in the unknowns $\rho, \mathbf{x}, \theta$, with $\dot{\mathbf{x}} = \mathbf{v}$. The system is of parabolic character in that it involves the highest order through the terms $\nabla \nabla \nabla \rho$ and $\nabla \Delta \rho$. To give evidence to the parabolic character consider possible third-order discontinuity waves ([7], §175) where

(1) At any time $t \in \mathbb{R}$ the third-order and all higher-order derivatives of $\rho, \mathbf{x}, \theta$ suffer jump discontinuities across a time-dependent surface $\sigma(t) \in \Omega$ but are continuous everywhere else;
(2) The functions $\rho, \mathbf{x}, \theta$ and their derivatives up to second order are continuous functions across $\sigma(t)$.

Let $[\![\cdot]\!]$ denote the jump of a quantity across σ. If, for formal simplicity, we consider a one-dimensional setting so that σ is a plane wave moving along the x direction, we find the jump condition

$$0 = (2\xi \partial_\xi^2 \hat{\psi} + \partial_\xi \hat{\psi}) \, [\![\partial_x^3 \rho]\!]$$

while the other relations are satisfied identically. It follows that

$$[\![\partial_x^3 \rho]\!] = 0.$$

This indicates that a more realistic model of the Korteweg type should maintain the dependence of the stress on the second-order density gradients but, at the same time, should contain suitable time derivatives so that the wave propagation condition is satisfied. The intrinsic features of the Korteweg fluid, namely the dependence of the stress tensor on the second-order derivatives of the mass density, would be conserved by letting the added terms vanish in stationary conditions.

The structure (39) shows that the stress tensor $\mathbf{T}$ is the sum of an isotropic term and a dyadic dependence $\nabla \rho \otimes \nabla \rho$. Hence, the boundary condition between a Korteweg fluid and, e.g., a rarefied gas modelled as an ideal gas would require the continuity of $\mathbf{Tn}$ and hence the vanishing of $(\nabla\rho \cdot \mathbf{n})\nabla\rho$. This in turn is satisfied by the vanishing of the normal derivative $\nabla\rho \cdot \mathbf{n}$.

7. A Fluid Model with Second-Order Space and Time Derivatives

The Korteweg fluid and the model of quantum hydrodynamics is based on a stress tensor which is linear in the second-order density gradient. While the dependence on second-order gradients is often motivated by the modelling of nanosystems, an analogous dependence on time derivatives might be required to account for propagation properties. It is worth remarking that hyperbolicity is mainly motivated by the conceptual requirement of finite wave speed along with the fit of experimental wave speeds. It may happen though that parabolic equations sometimes allow a better fit of wave profiles.

In essence, the Korteweg stress tensor comprises a dependence on $\nabla\nabla\rho$ and we look for an additional dependence on $\ddot{\rho}$. We recall that a dependence on the second-order time derivative of the strain occurs in the Burgers fluid model (see, [12], §6.4.1) but this is framed within a relation for the second-order rate of the stress. Hence, a different scheme is in order. Further, we try to establish a thermodynamic derivation so that the possible result would be thermodynamically consistent.

For the sake of simplicity, we neglect heat conduction and then the entropy inequality is written in the form

$$-\rho(\dot{\psi} + \eta\dot{\theta}) + \mathbf{T} \cdot \mathbf{D} + \theta\nabla \cdot \mathbf{k} = \rho\theta\gamma \geq 0. \tag{40}$$

Still, we let

$$\mathbf{T} = -p\mathbf{1} + \boldsymbol{\mathcal{T}},$$

where p is the thermodynamic pressure and then has to be determined through the thermodynamic analysis.

Hence, we set up a thermodynamic scheme where

$$\Gamma = (\theta, \rho, \nabla\rho, \dot{\rho}, \nabla\nabla\rho, \ddot{\rho}, \mathbf{D})$$

is the set variables. The stress tensor $\mathbf{T} = -p\mathbf{1} + \boldsymbol{\mathcal{T}}$, the entropy η, the entropy flux $\mathbf{k}$, and the entropy production γ are continuous functions of Γ, and the free energy ψ is continuously differentiable. Upon computation of $\dot{\psi}$ and substitution in (40), we have

$$\begin{aligned} -\rho(\partial_\theta\psi + \eta)\dot{\theta} - \rho\partial_\rho\psi\dot{\rho} - \rho\partial_{\nabla\rho}\psi \cdot (\nabla\rho)^{\cdot} - \rho\partial_{\dot{\rho}}\psi\ddot{\rho} - \rho\partial_{\nabla\nabla\rho}\psi \cdot (\nabla\nabla\rho)^{\cdot} - \rho\partial_{\ddot{\rho}}\psi\,\dddot{\rho} \\ -\rho\partial_{\mathbf{D}}\psi \cdot \dot{\mathbf{D}} - p\nabla \cdot \mathbf{v} + \boldsymbol{\mathcal{T}} \cdot \mathbf{D} + \theta\nabla \cdot \mathbf{k} = \rho\theta\gamma \geq 0. \end{aligned} \tag{41}$$

We first notice that $\dddot{\rho}$, $(\nabla\nabla\rho)^{\cdot}$, and $\dot{\mathbf{D}}$ occur linearly in (41) and can take arbitrary values. Hence, it follows that

$$\partial_{\ddot{\rho}}\psi = 0, \qquad \partial_{\nabla\nabla\rho}\psi = 0, \qquad \partial_{\mathbf{D}}\psi = 0.$$

Further, the linearity and arbitrariness of $\dot{\theta}$ imply that

$$\eta = -\partial_\theta\psi.$$

We cannot conclude that $\partial_{\dot{\rho}}\psi = 0$ in that $\mathbf{T}, \mathbf{k}$, and γ are allowed to depend on $\ddot{\rho}$. Indeed, based on the aim of obtaining the result that $\mathbf{T}$ depends on $\ddot{\rho}$, we assume

$$\partial_{\dot{\rho}}\psi = \alpha(\theta, \rho)\dot{\rho}. \tag{42}$$

Divide the remaining inequality by θ and replace $\dot{\rho}$ with $-\rho\nabla \cdot \mathbf{v}$ to obtain

$$\frac{1}{\theta}[\rho^2\partial_\rho\psi + \alpha\rho\ddot{\rho} - p]\nabla \cdot \mathbf{v} - \frac{\rho}{\theta}\partial_{\nabla\rho}\psi \cdot (\nabla\rho)^{\cdot} + \frac{1}{\theta}\boldsymbol{\mathcal{T}} \cdot \mathbf{D} + \nabla \cdot \mathbf{k} = \rho\gamma.$$

Using the identities

$$(\nabla\rho)^{\cdot} = \nabla\dot{\rho} - \mathbf{L}^T\nabla\rho = \nabla\dot{\rho} - \mathbf{D}\nabla\rho + \mathbf{W}\nabla\rho$$

$$-\frac{\rho}{\theta}\partial_{\nabla\rho}\psi \cdot \nabla\dot{\rho} = -\nabla\cdot[\frac{\rho}{\theta}\partial_{\nabla\rho}\psi\,\dot{\rho}] + [\nabla\cdot(\frac{\rho}{\theta}\partial_{\nabla\rho}\psi]\dot{\rho}$$

we can write

$$\frac{1}{\theta}[\rho^2\delta_\rho\psi + \alpha\rho\ddot{\rho} - p]\nabla\cdot\mathbf{v} + \frac{\rho}{\theta}(\nabla\rho\otimes\partial_{\nabla\rho}\psi)\cdot\mathbf{W} + \frac{1}{\theta}[\boldsymbol{\mathcal{T}} + \rho\nabla\rho\otimes\partial_{\nabla\rho}\psi]\cdot\mathbf{D}$$
$$+\nabla\cdot[\mathbf{k} - \frac{\rho}{\theta}\partial_{\nabla\rho}\psi\dot{\rho}] = \rho\gamma \geq 0.$$

Consequently, apart from a useless divergence-free term, we can take the entropy flux $\mathbf{k}$ in the form

$$\mathbf{k} = \frac{\rho}{\theta}\partial_{\nabla\rho}\psi\dot{\rho}.$$

The linearity and the skew symmetry of $\mathbf{W}$ imply that

$$(\nabla\rho\otimes\partial_{\nabla\rho}\psi) \in \mathrm{Sym}, \qquad \partial_{\nabla\rho}\psi \propto \nabla\rho. \tag{43}$$

To distinguish the contributions of the pressure p from that of $\mathrm{tr}\,\boldsymbol{\mathcal{T}}$, we assume p is independent of $\nabla\cdot\mathbf{v}$ and let

$$p = \rho^2\delta_\rho\psi + \alpha\rho\ddot{\rho}. \tag{44}$$

In light of (43), we let

$$\partial_{\nabla\rho}\psi = \beta\,\nabla\rho$$

and let β depend on θ and ρ. The remaining inequality

$$[\boldsymbol{\mathcal{T}} + \rho\nabla\rho\otimes\partial_{\nabla\rho}\psi]\cdot\mathbf{D} \geq 0$$

implies that

$$\boldsymbol{\mathcal{T}} = -\rho\beta\nabla\rho\otimes\nabla\rho + O(\mathbf{D}).$$

Indeed, the inequality holds with a nonzero stretching tensor $\mathbf{D}$ if, e.g., the Navier–Stokes constitutive equation is generalized in the form

$$\boldsymbol{\mathcal{T}} = -\rho\beta\nabla\rho\otimes\nabla\rho + 2\mu\mathbf{D} + \lambda(\mathrm{tr}\,\mathbf{D})1,$$

where $\mu \geq 0, \lambda + 2\mu/3 \geq 0$.

As a consequence of thermodynamics, the free energy is independent of $\ddot{\rho}, \nabla\nabla\rho$, and $\mathbf{D}$ so that

$$\psi = \psi(\theta,\rho,\nabla\rho,\dot{\rho}).$$

Further, as with the Korteweg model, the assumed isotropy of the fluid implies that ψ depends on $\nabla\rho$ through $|\nabla\rho|$ and hence for formal convenience we keep the dependence on $\xi = \frac{1}{2}|\nabla\rho|^2$. Moreover, by (42), it follows

$$\psi(\theta,\rho,\nabla\rho,\dot{\rho}) = \psi_0(\theta,\rho,\xi) + \tfrac{1}{2}\alpha(\theta,\rho)\dot{\rho}^2.$$

Consequently, the free energy involves only the first-order derivatives $\nabla\rho$ and $\dot{\rho}$ of the mass density.

7.1. The Detailed Structure of the Stress Tensor

In the Korteweg model of fluid, as well as in the present model, the stress $\boldsymbol{\mathcal{T}}$ comprises a dissipative part (the classical Navier–Stokes part $2\mu\mathbf{D} + \lambda(\mathrm{tr}\,\mathbf{D})1$) and a conservative part

$$-\rho\partial_\xi\psi\nabla\rho\otimes\nabla\rho.$$

As is apparent, the dependence on the derivatives is only through the gradient $\nabla\rho$. This stress is induced by the dyadic product $\nabla\rho \otimes \nabla\rho$ and is related to the free energy through the partial derivative $\partial_\xi \psi$.

Things are more involved with the pressure p. First, observe that the new term $\alpha\rho\ddot{\rho}$ is linear in $\ddot{\rho}$ and is related to the free energy in that $\alpha = \partial_{\dot{\rho}}\psi/\dot{\rho}$ though ψ is independent of $\ddot{\rho}$. The other term, $\rho^2\delta_\rho\psi$, is common to the Korteweg fluid. For definiteness, let

$$\psi = \Psi(\theta, \rho) + \hat{\psi}(\xi) + \tfrac{1}{2}\alpha\dot{\rho}^2.$$

It follows

$$\begin{aligned} p &= \rho^2\delta_\rho\psi + \alpha\rho\ddot{\rho} \\ &= \rho^2\partial_\rho\Psi + \tfrac{\rho^2}{\theta}\partial_\xi\hat{\psi}\nabla\theta\cdot\nabla\rho - \tfrac{1}{\rho}\partial_\xi\hat{\psi}|\nabla\rho|^2 - \rho^2\partial^2_\xi\hat{\psi}(\nabla\rho\otimes\nabla\rho)\cdot\nabla\nabla\rho - \rho^2\partial_\xi\hat{\psi}\Delta\rho + \alpha\rho\ddot{\rho}. \end{aligned}$$

7.2. Dynamics and Discontinuity Waves

For a simple check of the present model we assume the fluid is inviscid ($\mu = 0, \lambda = 0$). Hence, the dynamic equations are

$$\left\{ \begin{array}{l} \dot{\rho} = -\rho\nabla\cdot\mathbf{v}, \\ \rho\dot{\mathbf{v}} = -\nabla p - \nabla\cdot(\rho\partial_\xi\hat{\psi}\nabla\rho\otimes\nabla\rho) + \rho\mathbf{b}, \\ \rho\dot{\varepsilon} = -p\nabla\cdot\mathbf{v} - \rho\partial_\xi\hat{\psi}(\nabla\rho\otimes\nabla\rho)\cdot\mathbf{D} + \rho r. \end{array} \right. \tag{45}$$

Further, to avoid lengthy calculations, we select $\hat{\psi} = \varkappa\xi$ and hence

$$\partial_\xi\hat{\psi} = \varkappa, \qquad \partial^2_\xi\hat{\psi} = 0.$$

Consequently,

$$p = \rho^2\partial_\rho\Psi + \varkappa\frac{\rho^2}{\theta}\nabla\theta\cdot\nabla\rho - \frac{2\varkappa}{\rho}\xi - \varkappa\rho^2\Delta\rho + \alpha\rho\ddot{\rho}.$$

Notice that

$$\nabla\xi = (\nabla\rho\cdot\nabla)\nabla\rho.$$

Thus, we have

$$\begin{aligned} \nabla p = \nabla(\rho^2\partial_\rho\Psi + \varkappa\frac{\rho^2}{\theta}\nabla\theta\cdot\nabla\rho) + \frac{2\varkappa}{\rho^2}\xi\nabla\rho - \frac{2\varkappa}{\rho}(\nabla\rho\cdot\nabla)\nabla\rho - 2\varkappa\rho\Delta\rho\,\nabla\rho + \alpha\ddot{\rho}\,\nabla\rho \\ -\varkappa\rho^2\nabla\Delta\rho + \alpha\rho\nabla\ddot{\rho}, \end{aligned}$$

$$\nabla\cdot(\rho\partial_\xi\hat{\psi}\nabla\rho\otimes\nabla\rho) = \nabla(\varkappa\rho\nabla\rho\otimes\nabla\rho) = 2\varkappa\,\xi\,\nabla\rho + \varkappa\rho(\nabla\rho\cdot\nabla)\nabla\rho + \varkappa\rho\nabla\rho\,\Delta\rho,$$

and

$$\varepsilon = (\Psi - \theta\partial_\theta\Psi)(\theta, \rho) + \varkappa\xi + \tfrac{1}{2}\alpha\dot{\rho}^2.$$

Third-Order Discontinuity Waves

Relative to the unknowns $\rho, \mathbf{x}, \theta$, the system (45) shows that the highest-order derivatives are $\nabla\Delta\rho$ and $\nabla\ddot{\rho}$ which occur in ∇p. We then look for third-order discontinuity wave solutions by assuming that:

(1) At any time $t \in \mathbb{R}$, the third-order and all higher-order derivatives of $\rho, \mathbf{x}, \theta$ suffer jump discontinuities across a time-dependent surface $\sigma(t) \in \Omega$ but are continuous everywhere else;

(2) The functions $\rho, \mathbf{x}, \theta$ and their derivatives up to second order are continuous functions across $\sigma(t)$.

We denote by $[\![\cdot]\!]$ the pertinent jump across σ, and observe that the first and third equations of the system (45) result in two identities while the second equation yields

$$0 = -\varkappa\rho^2[\![\nabla\Delta\rho]\!] + \alpha\rho[\![\nabla\ddot{\rho}]\!]. \tag{46}$$

Observe that $\nabla\Delta\rho = \Delta\nabla\rho$, ahead of and behind σ, but

$$\nabla\ddot{\rho} \neq (\nabla\rho)^{\cdot\cdot}.$$

Now, by direct computation of $\nabla\ddot{\rho}$ (see Appendix A), we find that, if $\nabla\rho, \mathbf{v}, \partial_t\mathbf{v}, \mathbf{L}$ vanish, ahead of and then behind σ, it follows

$$[\![\nabla\ddot{\rho}]\!] = [\![\nabla\partial_t^2\rho]\!] = [\![\partial_t^2\nabla\rho]\!].$$

Since $[\![\nabla\rho]\!] = 0$, then the geometrical and kinematical conditions of compatibility (see, e.g., [8], ch. 6) yield

$$[\![\Delta\nabla\rho]\!] = [\![\partial_n^2\nabla\rho]\!], \qquad [\![\partial_t^2\nabla\rho]\!] = u^2[\![\partial_n^2\nabla\rho]\!],$$

where ∂_n is the normal derivative and u is the speed of propagation of σ. Thus, Equation (46) results in

$$(-\varkappa\rho + \alpha u^2)[\![\partial_n^2\nabla\rho]\!] = 0.$$

Non-trivial discontinuities occur with speed of propagation

$$u^2 = \frac{\varkappa\rho}{\alpha}.$$

8. Constitutive and Dynamic Equations in Incompressible Flows

A simpler, practical case is obtained by restricting the model to incompressible flows; a similar model is examined in [21] through an implicit relation for the Cauchy stress. We assume

$$\dot{\rho} = 0, \ \nabla\cdot\mathbf{v} = 0,$$

but, to maintain the interest in a Korteweg-type stress, we let

$$\nabla\rho \neq 0.$$

The coexistence of $\dot{\rho} = 0$ and $\nabla\rho \neq 0$ suggests that we review briefly the thermodynamic derivation.

Notice that $\operatorname{tr}\mathbf{D} = \nabla\cdot\mathbf{v} = 0$ and hence $\mathbf{D} = \mathbf{D}_0$. The pressure p is assumed to be given by a function of θ and ρ. Hence, we let

$$\boldsymbol{\mathcal{T}} := \mathbf{T} + p(\theta,\rho)1.$$

Let $(\theta, \rho, \nabla\theta, \nabla\rho, \mathbf{D}_0)$ be the set of variables. The Clausius–Duhem inequality reads

$$\begin{aligned} -\rho(\partial_\theta\psi + \eta)\dot{\theta} - \rho\partial_{\nabla\theta}\psi\cdot(\nabla\theta)^{\cdot} - \rho\partial_{\nabla\rho}\psi\cdot(\nabla\rho)^{\cdot} - \rho\partial_{\nabla\nabla\rho}\psi\cdot(\nabla\nabla\rho)^{\cdot} - \rho\partial_{\mathbf{D}_0}\psi\cdot\dot{\mathbf{D}}_0 \\ + \boldsymbol{\mathcal{T}}\cdot\mathbf{D}_0 - \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta + \theta\nabla\cdot\mathbf{k} = \rho\theta\gamma \geq 0. \end{aligned} \tag{47}$$

The linearity and arbitrariness of $\dot{\theta}, (\nabla\theta)^{\cdot}, \dot{\mathbf{D}}_0$ imply

$$\partial_{\nabla\theta}\psi = 0, \quad \partial_{\mathbf{D}_0}\psi = 0, \quad \eta = -\partial_\theta\psi.$$

Notice that, since $\nabla\cdot\mathbf{v} = 0$, we have

$$(\nabla\nabla\rho)^{\cdot} = -\mathbf{L}^T\nabla\otimes\nabla\rho - \nabla\otimes\mathbf{L}^T\nabla\rho;$$

the arbitrariness of $(\nabla\nabla\rho)^{\cdot}$ then implies that

$$\partial_{\nabla\nabla\rho}\psi = 0.$$

Since now $\mathbf{k}$ is independent of $\dot{\rho}$, then no generality is lost by assuming $\mathbf{k} = 0$. Hence, inequality (47) simplifies to

$$\boldsymbol{\mathcal{T}} \cdot \mathbf{D}_0 + \rho(\nabla\rho \otimes \partial_{\nabla\rho}\psi) \cdot (\mathbf{D}_0 + \mathbf{W}) - \frac{1}{\theta}\mathbf{q} \cdot \nabla\theta = \rho\theta\gamma \geq 0. \tag{48}$$

The arbitrariness of $\mathbf{W} \in \mathrm{Skw}$ implies

$$\nabla\rho \otimes \partial_{\nabla\rho}\psi \in \mathrm{Sym}, \quad \partial_{\nabla\rho}\psi \parallel \nabla\rho, \quad \psi = \psi(\theta, \xi), \quad \xi = \tfrac{1}{2}|\nabla\rho|^2.$$

If $\boldsymbol{\mathcal{T}}$ is assumed to be independent of $\nabla\theta$, then it follows from (48) that

$$\mathbf{T} = -p(\theta,\rho)1 - \rho\partial_\xi\psi\nabla\rho \otimes \nabla\rho + \mu\mathbf{D}_0, \qquad \mu \geq 0$$

$$\mathbf{q} \cdot \nabla\theta = -\rho\theta^2\gamma_q$$

where $\rho\theta\gamma_q = \rho\theta\gamma - \mu\mathbf{D}_0 \cdot \mathbf{D}_0 \geq 0$.

The evolution equations consist of the equations of motion and of the balance of energy. To compute $\nabla \cdot \mathbf{T}$, we notice that

$$\nabla \cdot (\rho\partial_\xi\psi\nabla\rho \otimes \nabla\rho) = [(\partial_\xi\psi + \rho\partial^2_\xi\psi)|\nabla\rho|^2 + \rho\partial_\xi\psi\Delta\rho]\nabla\rho + \rho\partial_\xi\psi(\nabla\nabla\rho)\nabla\rho$$

while to represent the balance of energy we employ the relations

$$\mathbf{T} \cdot \mathbf{D}_0 = -\rho\partial_\xi\psi(\nabla\rho \otimes \nabla\rho) \cdot \mathbf{D}_0 + \mu\mathbf{D}_0 \cdot \mathbf{D}_0,$$

$$\partial_\theta\varepsilon = \theta\partial_\theta\eta,$$

$$\dot{\xi} = (\tfrac{1}{2}|\nabla\rho|^2)^{\cdot} = -(\nabla\rho \otimes \nabla\rho) \cdot \mathbf{D}_0.$$

We can then write the evolution equations in the form

$$\rho\dot{\mathbf{v}} = -\nabla p(\theta,\rho) - [(\partial_\xi\psi + \rho\partial^2_\xi\psi)|\nabla\rho|^2 + \rho\partial_\xi\psi\Delta\rho]\nabla\rho - \rho\partial_\xi\psi(\nabla\nabla\rho)\nabla\rho + \mu\nabla \cdot \mathbf{D}_0 + \rho\mathbf{b},$$

$$\rho\theta\partial_\theta\eta\dot{\theta} = \rho\theta\partial_\xi\eta(\nabla\rho \otimes \nabla\rho) \cdot \mathbf{D}_0 - \nabla \cdot \mathbf{q} + \rho r.$$

9. Conclusions

This paper addresses materials with constitutive equations embodying higher-order gradients. The motivation for this topic arises from two remarkable schemes where the constitutive equation for the stress tensor involves higher-order gradients of the mass density. Within continuum mechanics this is the case of the Korteweg fluid. In quantum hydrodynamics this dependence follows from the assumption of the quantum potential in the form that traces back to Bohm. In this paper, we have reviewed the derivation of both stress tensors.

Next, we have investigated the thermodynamic consistency of stress tensors with dependencies on density gradients up to second order. The results (32) and (34) give possible constitutive equations for the stress tensor with second-order gradients. It is an advantage of this general approach that the coefficients of the representation are appropriate functions of ρ and θ, determined by a thermodynamic potential, here $\psi(\theta,\rho,\xi)$, $\xi = \frac{1}{2}|\nabla\rho|^2$. This in turn allows the coefficients to be related to a single potential function.

A detailed comparison with previous results is made, both with the Korteweg-type stress and the quantum stress. The connection is also established with other approaches, namely, that involving the interstitial working [11] and that applying Liu's procedure for the Clausius–Duhem inequality [10]. A direct application of thermodynamic requirements to quantum hydrodynamics shows open questions for future developments.

Finally, upon the observation that Korteweg-type stress tensors are not compatible with wave propagation, at a finite speed, an improvement of the model is attempted so that the finite speed occurs in a thermodynamically consistent model. The thermodynamic approach shows that an additive term $\alpha\rho\ddot{\rho}$ of the pressure is allowed. Though more refined improvements might be desirable, it follows that this additive term of the pressure allows the propagation of third-order discontinuity waves, $[\![\nabla\nabla\nabla\rho]\!] \neq 0$, and allows the recovery of the Korteweg stress tensor in stationary conditions.

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Appendix A

Representation of $(\nabla g)^{\cdot}$ and $(\nabla\nabla g)^{\cdot}$.

To prove the identities (17), (18) it is convenient to use the suffix notation. By definition, if $g \in C^2(\Omega \times \mathbb{R})$, then

$$\begin{aligned}(\partial_{x_i} g)^{\cdot} &= \partial_t \partial_{x_i} g + v_k \partial_{x_k} \partial_{x_i} g \\ &= \partial_{x_i} \partial_t g + v_k \partial_{x_i} \partial_{x_k} g \\ &= \partial_{x_i} \partial_t g + \partial_{x_i}(v_k \partial_{x_k} g) - (\partial_{x_i} v_k)\partial_{x_k} g \\ &= \partial_{x_i} \dot{g} - L_{ki} \partial_{x_k} g\end{aligned}$$

whence (17) follows.

Likewise, if $g \in C^3(\Omega \times \mathbb{R})$, we compute

$$\begin{aligned}(\partial_{x_i}\partial_{x_j} g)^{\cdot} &= (\partial_t + v_k \partial_{x_k})\partial_{x_i}\partial_{x_j} g \\ &= \partial_{x_i}\partial_{x_j}\partial_t g + v_k \partial_{x_i}\partial_{x_j}\partial_{x_k} g \\ &= \partial_{x_i}\partial_{x_j}\partial_t g + \partial_{x_i}(v_k \partial_{x_j}\partial_{x_k} g) - (\partial_{x_i} v_k)(\partial_{x_j}\partial_{x_k} g) \\ &= \partial_{x_i}\partial_{x_j}\partial_t g + \partial_{x_i}\partial_{x_j}(v_k \partial_{x_k} g) - \partial_{x_i}[(\partial_{x_j} v_k)\partial_{x_k} g] - (\partial_{x_i} v_k)(\partial_{x_j}\partial_{x_k} g) \\ &= \partial_{x_i}\partial_{x_j}(\partial_t g + v_k \partial_{x_k} g) - \partial_{x_i}[L_{kj}\partial_{x_k} g] - (\partial_{x_i} v_k)(\partial_{x_j}\partial_{x_k} g)\end{aligned}$$

to obtain

$$(\partial_{x_i}\partial_{x_j} g)^{\cdot} = \partial_{x_i}\partial_{x_j}\dot{g} - \partial_{x_i}(L^T_{jk}\partial_{x_k} g) - (L^T_{ik}\partial_{x_k})\partial_{x_j} g.$$

Replacing $g = \rho$ and $\dot{\rho} = -\rho\nabla \cdot \mathbf{v}$, we have

$$\begin{aligned}(\partial_{x_i}\partial_{x_j} g)^{\cdot} = -(\partial_{x_i}\partial_{x_j}\rho)\nabla \cdot \mathbf{v} - 2\partial_{x_i}\rho\, \partial_{x_j}\nabla \cdot \mathbf{v} - \rho\partial_{x_i}\partial_{x_j}\nabla \cdot \mathbf{v} \\ -(\partial_{x_i}\partial_{x_j} v_k)\partial_{x_k}\rho - L^T_{jk}\partial_{x_i}\partial_{x_k}\rho - L^T_{ik}\partial_{x_j}\partial_{x_k}\rho\end{aligned}$$

and the expression (18) follows.

Representation of $\nabla\ddot{g}$.

Notice that

$$\begin{aligned}\ddot{g} &= (\partial_t + \mathbf{v} \cdot \nabla)(\partial_t g + \mathbf{v} \cdot \nabla g) \\ &= \partial_t^2 g + \partial_t(\mathbf{v} \cdot \nabla g) + (\mathbf{v} \cdot \nabla)\partial_t g + (\mathbf{v} \cdot \nabla)(\mathbf{v} \cdot \nabla g) \\ &= \partial_t^2 g + \partial_t \mathbf{v} \cdot \nabla g + 2\mathbf{v} \cdot \partial_t \nabla g + \nabla g \cdot \mathbf{L}\mathbf{v} + (\mathbf{v} \otimes \mathbf{v}) \cdot \nabla\nabla g\end{aligned}$$

or

$$\ddot{g} = \partial_t^2 g + (\partial_t v_j)\partial_{x_j} g + 2v_i \partial_{x_i} \partial_t g + (\partial_{x_j} g) L_{ji} v_i + v_i v_j \partial_{x_i} \partial_{x_j} g.$$

Hence, we obtain

$$\begin{aligned}\partial_{x_k} \ddot{g} = \partial_t^2 \partial_{x_k} g + (\partial_t \partial_{x_k} v_j)\partial_{x_j} g + (\partial_t v_j)\partial_{x_j} \partial_{x_k} g + 2(\partial_{x_k} v_i)\partial_t \partial_{x_i} g + 2v_i \partial_t \partial_{x_i} \partial_{x_k} g \\ +(\partial_{x_j} \partial_{x_k} g) L_{ji} v_i + (\partial_{x_j} g)(\partial_{x_i} \partial_{x_k} v_j) v_i + (\partial_{x_j} g) L_{ji} \partial_{x_k} v_i \\ +(\partial_{x_k} v_i) v_j \partial_{x_i} \partial_{x_j} g + v_i (\partial_{x_k} v_j)\partial_{x_i} \partial_{x_j} g + v_i v_j (\partial_{x_k} \partial x_i \partial_{x_j} g).\end{aligned}$$

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