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MATHEMATICAL MODELING OF ELASTIC PHASE TRANSITIONS

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Various modifications are proposed for a model describing phase transitions in multidimensional elastic media via a nonconvex free energy function. The material density is considered to be an order parameter responsible for the difference between phases. These models can be used in the description of physical phenomena, such as phase transitions in solids (e.g., graphite–diamond), or in the description of shape-memory materials. In the case of one space variable, the model is a generalization of the well-known Falk model [1–3]. Some of its partial solutions are found.

1. Introduction. It is agreed that a *phase transition* takes place if some of the quantities that characterize macroscopic properties of a material change discontinuously with respect to external variables. The energy function is used as one of the parameters to describe the state of the material. This may be the internal energy, the Helmholtz free energy, or the Gibbs free energy which are connected by the Legendre transform. We are interested not in the well-known Stefan phase transitions when the energy of the material changes discontinuously, but in the transitions for which the energy function varies continuously, and its derivatives may have a discontinuity. If the first derivatives are discontinuous, then we have a *first-order* phase transition. For *second-order* phase, only the second derivatives may have a discontinuity. It is generally assumed that the internal energy and the Helmholtz free energy are nonconvex functions in some interval of their arguments. To describe phase transitions in more detail, we can use a specific parameter called the *order parameter* which characterizes the difference between phases.

The theoretical description of phase transitions started with the well-known van der Waals equation (see [4]) for the liquid–vapor first-order phase transition. In this work phase transitions were first described using a nonconvex energy function. In [5] dependence on the density gradient was added as a parameter to the free energy function to obtain a continuous profile across the liquid–vapor interface.

An important step in the description of the second-order phase transitions was taken by L. D. Landau [6] who began to develop the theory that was later referred to by his name. The basic assumption made in [6] is that the energy function only depends on the order parameter and temperature. To avoid the sharp distinction between phase boundaries, V. L. Ginzburg extended the energy function with the dependence on the gradient of the order parameter [7]. The differential equations thus obtained are often referred to as the Ginzburg–Landau phase transition theory. Independently, A. F. Devonshire [8] developed a similar theory for ferroelectrics.

In [1–3], strain is treated as the order parameter responsible for the phase difference in the description of the elastic phase transitions. In this case the free energy function is similar to that proposed in [6, 7]. The problems concerned with the one-dimensional Falk model were investigated in [9, 10].

Concerning the Falk models, we remark that they assume the material density to be constant, which is not always justified in practice.

2. The Static Landau Theory. Let a body occupy volume Ω and be in an equilibrium state. We study the equilibrium case when all the variables do not depend on time and the temperature θ is constant

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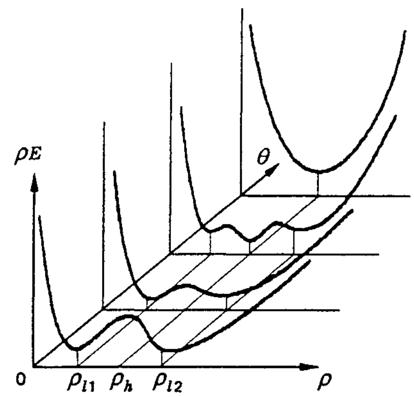

Fig. 1

throughout the volume Ω. The equilibrium state is determined by a minimum of total free energy

$$\mathcal{E} = \int_{\Omega} \rho E \, dx + \mathcal{E}_{\text{ext}} ,$$

where $\rho = \rho(\mathbf{x})$ is the material density; $\mathbf{x}$ are the space coordinates; ρE is the density of the Helmholtz free energy per unit volume; E is the specific free energy; $\mathcal{E}_{\text{ext}}$ is the contribution from the external forces to the total energy. In the Landau theory, we assume that E depends on the density ρ and temperature θ, and in the Ginzburg–Landau theory E depends also on the density gradient $\nabla\rho$. We do not refine the form of the function $\mathcal{E}_{\text{ext}}$, simply noting that $\mathcal{E}_{\text{ext}}$ is a functional of the displacement vector. For simplicity we can assume $\mathcal{E}_{\text{ext}} = 0$. This corresponds to the absence of external volumetric forces, and the domain boundary $\partial\Omega$ is also free from the action of the external surface forces, i.e., the body is free. A free body is in equilibrium if the equilibrium density ρ_{eq} represents the minimum of the function ρE.

For further consideration we postulate the equation of state as the dependence of E on ρ and θ. Assume that E, or more precisely, the function $F = \rho E$, is of a form similar to that presented in the picture: F is a nonconvex function of the argument ρ; $F \to \infty$ as $\rho \to 0$ and $\rho \to \infty$, F has the only minimum at high temperatures, which corresponds to the density ρ_h of the high temperature phase, and two (or more) minima at low temperatures corresponding to the densities ρ_{l_i} of the low temperatures phases. At some temperatures, high- and low-temperature phases may coexist.

An absolute minimum over ρ with the temperature fixed corresponds to the stable phase, and the other minima correspond to metastable phases. To decrease its energy, the material can change state from metastable to stable, but to do this it is necessary to overcome a certain energy barrier.

3. The Dynamic Landau Theory. The Lagrange description used thereafter is the most suitable for elastic bodies. We can write the system of equations for ρ, θ, and the displacement vector $\mathbf{u}$ using the equation of state $E = E(\rho, \theta)$. This is done in the same manner as in the thermoelasticity theory, with the only difference that in this theory $E = E(\hat{\varepsilon}, \theta)$, where $\hat{\varepsilon}$ is the Lagrange strain tensor

$$2\hat{\varepsilon} = \left(\frac{\partial \mathbf{u}}{\partial \boldsymbol{\xi}}\right)^* + \left(\frac{\partial \mathbf{u}}{\partial \boldsymbol{\xi}}\right) + \left(\frac{\partial \mathbf{u}}{\partial \boldsymbol{\xi}}\right)^* \circ \left(\frac{\partial \mathbf{u}}{\partial \boldsymbol{\xi}}\right), \quad \mathbf{u} = \mathbf{x} - \boldsymbol{\xi} \tag{3.1}$$

[$\boldsymbol{\xi}$ are the Lagrange coordinates, $\mathbf{x}$ are the Euler coordinates, $\mathbf{x} = \mathbf{x}(\boldsymbol{\xi}, t)$].

The formula for density can be derived from the equations of continuity and momentum [11]:

$$\rho(\boldsymbol{\xi}, t) = \rho_0(\boldsymbol{\xi})(1 + 2J_1 + 4J_2 + 8J_3)^{-1/2}. \tag{3.2}$$

Here $\rho_0(\boldsymbol{\xi})$ is the initial density distribution; $J_k = J_k(\hat{\varepsilon})$ is the kth invariant of the strain tensor $\hat{\varepsilon} = \hat{\varepsilon}(\boldsymbol{\xi}, t)$ ($k = 1, 2, 3$).

The internal energy U is connected with the free energy E, temperature θ, and entropy $\mathcal{S}$ by the relation $U = E + \theta\mathcal{S}$. It is convenient henceforth to denote by $\widehat{P}$ the auxiliary tensor connected with the stress tensor P by the formulas

$$P = T \circ \widehat{P} \circ T^*, \quad \widehat{P} = T^{-1} \circ P \circ T^{*-1}, \tag{3.3}$$

where

$$T = \frac{\partial \mathbf{x}}{\partial \boldsymbol{\xi}} = I + \frac{\partial \mathbf{u}}{\partial \boldsymbol{\xi}} \tag{3.4}$$

is the distortion tensor; I is the unit tensor.

Due to the elastic body thermodynamics axiom [11]

$$\rho\theta \frac{d\mathcal{S}}{dt} = \operatorname{div}(æ\nabla\theta) \tag{3.5}$$

we can derive

$$\widehat{P} = \rho \frac{\partial E}{\partial \rho} \frac{\partial \rho}{\partial \hat{\varepsilon}}, \qquad \mathcal{S} = -\frac{\partial E}{\partial \theta} \tag{3.6}$$

from the heat influx equation. Here $\partial\rho/\partial\hat{\varepsilon}$ is the gradient of the tensor function $\rho(\hat{\varepsilon})$ with respect to $\hat{\varepsilon}$.

Using (3.2) and (3.6), we find $\widehat{P}$:

$$\begin{aligned}
\widehat{P} &= -\rho \frac{\partial E}{\partial \rho}\left[\frac{1}{2}\rho_0(1 + 2J_1 + 4J_2 + 8J_3)^{-3/2}\, 2\left(\frac{\partial J_1}{\partial \hat{\varepsilon}} + 2\frac{\partial J_2}{\partial \hat{\varepsilon}} + 4\frac{\partial J_3}{\partial \hat{\varepsilon}}\right)\right] \\
&= -\rho \frac{\partial E}{\partial \rho} \frac{\rho^3}{\rho_0^2}[I + 2(J_1 I - \hat{\varepsilon}) + 4(J_2 I - J_1\hat{\varepsilon} + \hat{\varepsilon}^2)], \\
\widehat{P} &= -\frac{\rho^4}{\rho_0^2} \frac{\partial E}{\partial \rho}[(1 + 2J_1 + 4J_2)I - (2 + 4J_1)\hat{\varepsilon} + 4\hat{\varepsilon}^2].
\end{aligned} \tag{3.7}$$

The second formula in (3.6) and axiom (3.5) are used in deriving the equation for temperature

$$-\rho\theta \frac{\partial^2 E}{\partial \theta^2} \frac{\partial \theta}{\partial t} - \operatorname{div}(æ\nabla\theta) = \theta \frac{\partial \widehat{P}}{\partial \theta} : \frac{\partial \hat{\varepsilon}}{\partial t}. \tag{3.8}$$

Let us give an example of the dependence of E on θ:

$$\rho E(\rho, \theta) = E_0(\theta) + (\theta - \theta_0)E_1(\rho) + E_2(\rho), \quad E_0(\theta) = C_1 + C_2\theta - C\theta \ln\theta.$$

Here the coefficient at θ_t in Eq. (3.8) equals C. It would appear reasonable in the general case that

$$0 < -\rho\theta \frac{\partial^2 E}{\partial \theta^2} < \infty.$$

We insert the displacement $\mathbf{u}$ into the momental equation by the relations

$$\mathbf{v} = \frac{\partial \mathbf{x}}{\partial t} = \frac{\partial \mathbf{u}}{\partial t}, \quad \frac{d\mathbf{v}}{dt} = \frac{\partial^2 \mathbf{u}}{\partial t^2}.$$

The momrntal equation takes the form

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \operatorname{div} P + \rho \mathbf{f}. \tag{3.9}$$

It is easy to verify that Eqs. (3.8) and (3.9) together with Eqs. (3.1)-(3.4), and (3.7) form a closed system of equations for $\mathbf{u}$ and θ. For the written form of the equations to be complete, it is necessary to change the div operations in (3.8) and (3.9) to the Lagrange coordinates. If div_x is written in the Euler coordinates, and div_ξ is written in the Lagrange coordinates (∇_x and ∇_ξ have the same meaning), then the transformation required is given by the formulas

$$\operatorname{div}_x P = \operatorname{div}_\xi(T \circ \widehat{P}) - T \circ \widehat{P} \circ T^*\langle \operatorname{div}_\xi(T^{*-1})\rangle; \tag{3.10}$$

$$\operatorname{div}_x(æ\nabla\theta) = \operatorname{div}_\xi(æT^{-1} \circ T^{*-1}\langle\nabla_\xi\theta\rangle) - æT^{*-1}\langle\nabla_\xi\theta\rangle \operatorname{div}_\xi(T^{*-1}). \tag{3.11}$$

System (3.1)–(3.4), (3.7)–(3.11) is complicated both for solving particular problems and for the general mathematical analysis. For this reason we study its linear variant.

The starting point of the linear theory is the notion of a natural state of a thermoelastic body. A state is called natural if there are no deformations ($\hat{\varepsilon} = 0$) in it, and the density and temperature are constants ($\rho = \rho_0$, $\theta = \theta_0$). We search for another solution which differs little from the natural state. A deformation is called small if the norm of the tensor $T - I$ is small in comparison with the units. According to formulas (3.1) and (3.4), smallness of deformations is equivalent to smallness of the norm of the tensor $\partial\mathbf{u}/\partial\boldsymbol{\xi}$ or $\hat{\varepsilon}$. In addition, we assume that the temperature difference $\tilde{\theta} = \theta - \theta_0$ and its derivatives are small (of the order of smallness of the tensor $\hat{\varepsilon}$). We obtain the relationships of the linear theory if we drop the quantities of the highest order of smallness in comparison with a small norm of the tensor $T - I$. Thus, according to the linear theory, relations (3.1) and (3.2) are reduced to the following:

$$2\hat{\varepsilon} = \left(\frac{\partial\mathbf{u}}{\partial\boldsymbol{\xi}}\right)^* + \left(\frac{\partial\mathbf{u}}{\partial\boldsymbol{\xi}}\right); \tag{3.12}$$

$$\rho = \rho_0(1 - J_1(\hat{\varepsilon})). \tag{3.13}$$

Formula (3.7) takes the form

$$\hat{P} = (-p - \alpha\tilde{\theta} + \lambda J_1)I + 2\mu\hat{\varepsilon}, \tag{3.14}$$

where

$$p = \mu = \rho_0^2 \frac{\partial E}{\partial \rho}(\rho_0, \theta_0); \qquad \alpha = \rho_0^2 \frac{\partial^2 E}{\partial\rho\partial\theta}(\rho_0, \theta_0); \quad \lambda = 2\rho_0^2 \frac{\partial E}{\partial \rho}(\rho_0, \theta_0) + \rho_0^3 \frac{\partial^2 E}{\partial \rho^2}(\rho_0, \theta_0).$$

When (3.14) is taken into account, the linearized Euler stress tensor P from (3.3) is written as

$$P = (-p - \alpha\tilde{\theta} + \lambda J_1)I. \tag{3.15}$$

Finally, we assume that the heat conductivity coefficient is $æ =$ const. As a result, Eqs. (3.8) and (3.9) are reduced to the following system of equations

$$\rho_0 \frac{\partial^2\mathbf{u}}{\partial t^2} = -\alpha\nabla\theta + \lambda\nabla(\operatorname{div}\mathbf{u}) + \rho_0\mathbf{f}; \tag{3.16}$$

$$\frac{\partial\theta}{\partial t} = k\Delta\theta - \beta\frac{\partial}{\partial t}(\operatorname{div}\mathbf{u}). \tag{3.17}$$

Here

$$k = \frac{æ}{-\rho_0\theta_0 \dfrac{\partial^2 E}{\partial\theta^2}(\rho_0, \theta_0)}; \qquad \beta = \frac{\alpha\theta_0}{-\rho_0\theta_0 \dfrac{\partial^2 E}{\partial\theta^2}(\rho_0, \theta_0)}.$$

The operations div, ∇, Δ in (3.16) and (3.17) are performed over the Lagrange variables $\boldsymbol{\xi}$ (for brevity, the index $\boldsymbol{\xi}$ is omitted).

Unlike the corresponding equations of the classical linear thermoelasticity theory, Eq. (3.16) has no term with $\Delta\mathbf{u}$. This is a fundamental point, since the remaining term $\lambda\nabla(\operatorname{div}\mathbf{u})$ is not an elliptic operator in the case of the stationary problem.

The initial conditions for Eqs. (3.16) and (3.17) have the form

$$\mathbf{u}\Big|_{t=0} = \mathbf{u}_0(\boldsymbol{\xi}), \quad \mathbf{u}_t\Big|_{t=0} = \mathbf{u}_1(\boldsymbol{\xi}), \quad \theta\Big|_{t=0} = \theta_0(\boldsymbol{\xi}), \tag{3.18}$$

and the boundary conditions on the side surface of the cylinder $S_T = \partial\Omega \times (0, T)$ are the following:

$$(\operatorname{div}\mathbf{u})\Big|_{S_T} = v_s(\boldsymbol{\xi}, t), \quad \theta\Big|_{S_T} = \theta_s(\boldsymbol{\xi}, t). \tag{3.19}$$

The problem (3.16)–(3.19) is well posed for $k > 0$, $\lambda > 0$, i.e., the solution $\{\mathbf{u}, \theta\}$ exists, is unique, and depends on the problem's data continuously. The proof of this statement is not given in this article.

In the case of one space variable $[(\xi,t)\in Q_T=(\xi_1,\xi_2)\times(0,T)]$, Eqs. (3.16) and (3.17) take the form

$$\rho_0 u_{tt} = -\alpha\theta_\xi + \lambda u_{\xi\xi} + \rho_c f; \tag{3.20}$$

$$\theta_t = k\theta_{\xi\xi} - \beta u_{\xi t}. \tag{3.21}$$

Let us consider the solutions of the problem (3.20), (3.21) with strong discontinuity, namely, it is assumed that there exists a smooth function $\xi = R(t)$ which divides the domain Q_T into two subdomains (Q_T^- and Q_T^+). In each of the subdomains Q_T^- and Q_T^+, functions u and θ are smooth functions and satisfy Eqs. (3.20) and (3.21) in the classical sense. The functions u, θ may have a discontinuity at the phase interface $\xi = R(t)$. In this case the jumps of the functions u, θ, u_ξ, and θ_ξ are not arbitrary but connected by definite relations called the strong discontinuity equations:

$$D[\rho_0 u_t] - [\alpha\theta] + [\lambda u_\xi] = 0; \tag{3.22}$$

$$D[\theta] + D[\beta u_\xi] + [k\theta_\xi] = 0. \tag{3.23}$$

Here $[g] = \lim\limits_{\xi\to R(t)+0} g(\xi,t) - \lim\limits_{\xi\to R(t)-0} g(\xi,t)$; D is the velocity of the boundary $\xi = R(t)$: $D = dR(t)/dt$; the coefficients ρ_0, α, λ, k, β are constants different in Q_T^- and Q_T^+.

We search for partial solutions with strong discontinuity in the infinite domain $(\xi,t)\in(-\infty,\infty)\times(0,\infty)$ which are of the type of running waves: $u(\xi,t) = u(\xi - at)$, $\theta(\xi,t) = \theta(\xi - at)$, $R(t) = at$. For this we assume that $\rho_0 f = \varphi(\xi - at)$ with the known function φ and given number a. Let us denote $\xi - at = z$, $u^- = u(z)$, $\theta^- = \theta(z)$ as $z < 0$, $u^+ = u(z)$, $\theta^+ = \theta(z)$ as $z > 0$. For functions $u^\pm$, $\theta^\pm$ from Eqs. (3.20) and (3.21) we have the system of ordinary differential equations:

$$a^2\rho_0 u_{zz} = -\alpha\theta_z + \lambda u_{zz} + \varphi; \tag{3.24}$$

$$-a\theta_z = k\theta_{zz} + a\beta u_{zz}, \tag{3.25}$$

and from the strong discontinuity equations (3.22) and (3.23) we have the conditions of conjugation for $z = 0$:

$$a^2[\rho_0 u_z] + [\alpha\theta] - [\lambda u_z] = 0; \tag{3.26}$$

$$a[\theta] + a[\beta u_z] + [k\theta_z] = 0 \tag{3.27}$$

($[g] = g^+(0) - g^-(0)$). On integrating the system (3.24), (3.25), we obtain

$$\theta^\pm(z) = \theta^\pm(0) + \theta_z^\pm(0)\,\frac{k^\pm}{A^\pm}\Big(1 - e^{-\frac{A^\pm}{k^\pm}z}\Big) - \frac{a\beta^\pm}{k^\pm(a^2\rho_0^\pm - \lambda^\pm)}\, e^{-\frac{A^\pm}{k^\pm}z}\int\limits_0^z e^{\frac{A^\pm}{k^\pm}y}\int\limits_0^y \varphi(x)\,dx\,dy,$$

$$u^\pm(z) = u^\pm(0) + \left(u_z^\pm(0) - \theta_z^\pm(0)\,\frac{k^\pm\alpha^\pm}{A^\pm(a^2\rho_0^\pm - \lambda^\pm)}\right)z + \theta_z^\pm(0)\,\frac{(k^\pm)^2\alpha^\pm}{(A^\pm)^2(a^2\rho_0^\pm - \lambda^\pm)}\Big(1 - e^{-\frac{A^\pm}{k^\pm}z}\Big)$$

$$+\frac{1}{(a^2\rho_0^\pm - \lambda^\pm)}\int\limits_0^z\int\limits_0^y \varphi(x)\,dx\,dy + \frac{a\alpha^\pm\beta^\pm}{k^\pm(a^2\rho_0^\pm - \lambda^\pm)^2}\int\limits_0^z e^{-\frac{A^\pm}{k^\pm}w}\int\limits_0^w e^{\frac{A^\pm}{k^\pm}y}\int\limits_0^y \varphi(x)\,dx\,dy\,dw,$$

$$A^\pm = a\left(1 - \frac{\alpha^\pm\beta^\pm}{(a^2\rho_0^\pm - \lambda^\pm)}\right).$$

Superscripts + and − correspond to the values with $z > 0$ and $z < 0$. Eight integration constants $[u^\pm(0)$, $u_z^\pm(0)$, $\theta^\pm(0)$, $\theta_z^\pm(0)]$ must meet two relations (3.26) and (3.27), and thus only six of them are independent, e.g., $u^\pm(0)$, $u_z^-(0)$, $\theta^\pm(0)$, $\theta_z^-(0)$. Then $u_z^+(0)$, $\theta_z^+(0)$ are found from (3.26) and (3.27).

4. The Dynamic Ginzburg–Landau Theory. It is assumed in the Ginzburg–Landau phase transition theory that the specific free energy E depends on the density ρ, temperature θ, and the density gradient $\nabla_\xi \rho = \rho_\xi = \Big(\partial\rho/\partial\xi_1, \partial\rho/\partial\xi_2, \partial\rho\partial\xi_3\Big)$:

$$E = E(\rho, \theta, \nabla_\xi\rho) = E_L(\rho,\theta) + \frac{\gamma}{2}\frac{|\nabla_\xi \rho|^2}{\rho} \tag{4.1}$$

[$E_L(\rho,\theta)$ is the Landau free energy].

The main problem of this section is to obtain the dependence of the Lagrange strain tensor $\widehat{P}$ on $\hat{\varepsilon}$ and θ which corresponds to the given function E from (4.1).

Let us consider an arbitrary movement of the domain Ω: $\hat{\varepsilon} = \hat{\varepsilon}(\xi, t)$, $\theta = \theta(\xi, t)$ satisfying the equation of the energy balance [11]:

$$\int\limits_{Q_T} \rho\frac{\partial U}{\partial t}\,d\xi dt = \int\limits_{Q_T} (\widehat{P} : \hat{\varepsilon}_t + \operatorname{div}(æ\nabla\theta))\,d\xi dt, \tag{4.2}$$

and the condition

$$\frac{\partial\rho}{\partial\mathbf{n}}\bigg|_{S_T} = \frac{\partial\rho}{\partial\xi}\cdot\mathbf{n}\bigg|_{S_T} = 0 \tag{4.3}$$

on the boundary $S_T = \partial\Omega\times(0,T)$ ($\mathbf{n}$ is the vector of the external normal to $\partial\Omega$).

Since $U(\xi,t) = E + \theta S$, we have

$$\rho\frac{\partial U}{\partial t} = \rho\frac{\partial E}{\partial t} + \rho\theta\frac{\partial S}{\partial t} + \rho S\frac{\partial\theta}{\partial t}; \tag{4.4}$$

$$\rho\frac{\partial E}{\partial t} = \rho\frac{\partial E}{\partial\rho}\frac{\partial\rho}{\partial t} + \rho\frac{\partial E}{\partial\theta}\frac{\partial\theta}{\partial t} + \rho\frac{\partial E}{\partial\rho_\xi}\frac{\partial\rho_\xi}{\partial t} = \rho\bigg(\frac{\partial E_L}{\partial\rho} - \frac{\gamma}{2\rho^2}|\nabla_\xi\rho|^2\bigg)\frac{\partial\rho}{\partial t} + \rho\frac{\partial E_L}{\partial\theta}\frac{\partial\theta}{\partial t} + \rho\Big(\frac{\gamma}{\rho}\rho_\xi\Big)\frac{\partial\rho_\xi}{\partial t}. \tag{4.5}$$

Substituting (4.4), (4.5) into (4.2) and using (3.5), we obtain

$$\int\limits_{Q_T}\bigg\{\bigg(\rho\frac{\partial E_L}{\partial\rho} - \frac{\gamma}{2\rho}|\nabla_\xi\rho|^2\bigg)\frac{\partial\rho}{\partial t} + \rho\bigg(\frac{\partial E_L}{\partial\theta} + S\bigg)\frac{\partial\theta}{\partial t}\bigg\}\,d\xi dt + \int\limits_{Q_T}\gamma\rho_\xi\frac{\partial\rho_\xi}{\partial t}\,d\xi dt = \int\limits_{Q_T}\widehat{P} : \hat{\varepsilon}_t\,d\xi dt. \tag{4.6}$$

We separately consider

$$\int\limits_{Q_T}\gamma\rho_\xi\frac{\partial\rho_\xi}{\partial t}\,d\xi dt = \gamma\int\limits_{Q_T}\bigg\{\operatorname{div}_\xi\Big(\rho_\xi\frac{\partial\rho}{\partial t}\Big) - \Delta_\xi\rho\frac{\partial\rho}{\partial t}\bigg\}\,d\xi dt = \gamma\int\limits_{S_T}\rho_\xi\cdot\mathbf{n}\frac{\partial\rho}{\partial t}\,d\xi dt - \gamma\int\limits_{Q_T}\Delta_\xi\rho\frac{\partial\rho}{\partial t}\,d\xi dt. \tag{4.7}$$

The integral over the boundary S_T from (4.7) equals zero due to condition (4.3). Taking into account $\partial\rho/\partial t = (\partial\rho/\partial\hat{\varepsilon}) : \hat{\varepsilon}_t$, we derive from (4.6) and (4.7)

$$\int\limits_{Q_T}\bigg\{\bigg(\rho\frac{\partial E_L}{\partial\rho} - \frac{\gamma}{2\rho}|\nabla_\xi\rho|^2 - \gamma\Delta_\xi\rho\bigg)\frac{\partial\rho}{\partial\hat{\varepsilon}} - \widehat{P}\bigg\} : \hat{\varepsilon}_t\,d\boldsymbol{\xi}dt + \int\limits_{Q_T}\rho\bigg(\frac{\partial E_L}{\partial\theta} + S\bigg)\frac{\partial\theta}{\partial t}\,d\boldsymbol{\xi}dt = 0. \tag{4.8}$$

Since $\hat{\varepsilon}$ and θ are independent and arbitrary, we have from (4.8)

$$S = -\frac{\partial E_L}{\partial\theta}, \quad \widehat{P} = \bigg(\rho\frac{\partial E_L}{\partial\rho} - \frac{\gamma}{2\rho}|\nabla_\xi\rho|^2 - \gamma\Delta_\xi\rho\bigg)\frac{\partial\rho}{\partial\hat{\varepsilon}}. \tag{4.9}$$

The quantity $\partial\rho/\partial\hat{\varepsilon}$ is already calculated when obtaining (3.7). The substitution of this expression into (4.9) results in the formula

$$\widehat{P} = \bigg(-\frac{\rho^4}{\rho_0^2}\frac{\partial E_L}{\partial\rho} + \frac{\gamma\rho^2}{2\rho_0^2}|\nabla_\xi\rho|^2 + \frac{\gamma\rho^3}{\rho_0^2}\Delta_\xi\rho\bigg)[(1 + 2J_1 + 4J_2)I - (2 + 4J_1)\hat{\varepsilon} + 4\hat{\varepsilon}^2]. \tag{4.10}$$

It is interesting to compare (4.10) with the expression for the stress tensor given by Korteweg [12] for compressible liquid:

$$K = \left(-\rho^2 \frac{\partial E}{\partial \rho} + c_1 |\nabla \rho|^2 + c_2 \Delta \rho \right) I + c_3 \nabla \rho \otimes \nabla \rho + c_4 \nabla \otimes \nabla \rho. \tag{4.11}$$

Here c_i are functions of the density ρ and temperature θ; $(\mathbf{a} \otimes \mathbf{b})_{ij} = a_i b_j$. It is clear that the terms with the unit tensor I in (4.10) and (4.11) are of the same kind.

Equations (3.8) and (3.9) together with formulas (3.1)–(3.4), and (4.10) form a closed system of equations for $\mathbf{u}$ and θ.

Acting as in Section 3, after linearization we obtain the linearized Lagrange stress tensor

$$\hat{P} = (-p - \alpha \tilde{\theta} + \lambda J_1 + \gamma \rho_0 \Delta \rho) I + 2\mu \hat{\varepsilon},$$

where p, α, λ, μ are the same as in formula (3.14) with E replaced by E_L. The linearized Euler stress tensor is $P = (-p - \alpha \tilde{\theta} + \lambda J_1 + \gamma \rho_0 \Delta \rho) I$.

Analogs of Eqs. (3.16) and (3.17) for $\mathbf{u}$ and θ take the form

$$\rho_0 \frac{\partial^2 \mathbf{u}}{\partial t^2} = -\alpha \nabla \theta + \lambda \nabla(\operatorname{div} \mathbf{u}) - \gamma \rho_0^2 \nabla \Delta(\operatorname{div} \mathbf{u}) + \rho_0 \mathbf{f}; \tag{4.12}$$

$$\frac{\partial \theta}{\partial t} = k \Delta \theta - \beta \frac{\partial}{\partial t}(\operatorname{div} \mathbf{u}). \tag{4.13}$$

Equations (4.12) and (4.13) have the following initial conditions:

$$\mathbf{u}\Big|_{t=0} = \mathbf{u}_0(\xi), \quad \mathbf{u}_t\Big|_{t=0} = \mathbf{u}_1(\xi), \quad \theta\Big|_{t=0} = \theta_0(\xi), \tag{4.14}$$

and the conditions on the side surface of the cylinder $S_T = \partial \Omega \times (0, T)$ are given by

$$(\operatorname{div} \mathbf{u})\Big|_{S_T} = 0, \quad \frac{\partial (\operatorname{div} \mathbf{u})}{\partial \mathbf{n}}\Big|_{S_T} = 0, \quad \theta\Big|_{S_T} = \theta_s(\xi, t). \tag{4.15}$$

The problem (4.12)–(4.15) is well posed.

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