Monatomic rarefied gas as a singular limit of polyatomic gas in extended thermodynamics

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ABSTRACT

We show that, in the theory of extended thermodynamics, rarefied monatomic gases can be identified as a singular limit of rarefied polyatomic gases. Under naturally conditioned initial data we prove that the system of 14 field equations for polyatomic gases in the limit has the same solutions as those of the system of 13 field equations for monatomic gases where there exists no dynamic pressure. We study two illustrative examples in the process of the limit, that is, the linear waves and the shock waves in order to grasp the asymptotic behavior of the physical quantities, in particular, of the dynamic pressure.

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1. Introduction and the statement of the problem

The applicability range of extended thermodynamics (ET) [1] is wider than that of thermodynamics of irreversible processes [2] basing on the local equilibrium assumption. On the other hand, however, ET of gases had been valid mainly for rarefied monatomic gases.

The prototype of ET corresponds to the kinetic moment theory by Grad [3], and it describes 13 independent fields, i.e., the mass density F, the momentum density F_i, the momentum flux F_{ij} and the energy flux F_{lli} satisfying the balance equations of the following type

$$\frac{\partial F}{\partial t} + \frac{\partial F_k}{\partial x_k} = 0,$$

$$\frac{\partial F_i}{\partial t} + \frac{\partial F_{ik}}{\partial x_k} = 0,$$

$$\frac{\partial F_{ij}}{\partial t} + \frac{\partial F_{ijk}}{\partial x_k} = P_{\langle ij \rangle},$$

$$\frac{\partial F_{lli}}{\partial t} + \frac{\partial F_{llik}}{\partial x_k} = P_{lli}, \tag{1}$$

where F_{ijk} and F_{llik} are the fluxes of F_{ij} and F_{lli}, respectively, and $P_{\langle ij \rangle}$ and P_{lli} are the productions of F_{ij} and F_{lli}, respectively. Here the angular brackets such as $P_{\langle ij \rangle}$ indicate that the corresponding tensor is a deviatoric (symmetric traceless) one. As the first five equations in the system (1) express the conservation laws of mass, momentum and energy, we have the relations

$$F = \rho, \qquad F_i = \rho v_i, \qquad F_{ij} = \rho v_i v_j - t_{ij},$$

$$F_{ll} = \rho v^2 + 2\rho\varepsilon, \qquad F_{lli} = \rho v^2 v_i - 2t_{il}v_l + 2q_i, \tag{2}$$

with the mass density ρ, the velocity v_i, the specific internal energy ε, the heat flux q_i, and the stress t_{ij}:

$$t_{ij} = -(p + \Pi)\delta_{ij} + S_{\langle ij \rangle}, \tag{3}$$

where p is the equilibrium pressure depending on ρ and ε, while Π and $S_{\langle ij \rangle}$ are, respectively, the dynamic pressure (nonequilibrium pressure) and the deviatoric shear stress.

In the hierarchy structure of the system (1), we notice two peculiarities: (i) the tensorial orders of the equations increase one by

one, and (ii) the flux of an equation becomes the density of the next equation. As a consequence, the trace of the momentum flux must be equal to the energy density. This implies that

$$3(p + \Pi) = 2\rho\varepsilon. \tag{4}$$

Then, as Π is a nonequilibrium quantity, we conclude that

$$3p = 2\rho\varepsilon, \qquad \Pi = 0. \tag{5}$$

In order to close the system (1) with respect to the independent variables ρ, v_i, ε, $S_{\langle ij \rangle}$ and q_i, the Grad approach [3] adopts a perturbative method derived from the kinetic theory, while ET adopts the constitutive equations restricted by the universal principles (*Entropy principle, Objectivity* and *Convexity*) [1]. Moreover the *maximum entropy principle* (MEP) [4] has also been utilized as a method of the closure in the case of 13 equations and generalized cases with many moments in [5]. The equivalence of MEP and the method of ET was proved [6].

Recently the present authors have proposed an ET theory of dense gases [7,8], where rarefied gases are included as a special case. The theory is applicable, in particular, to polyatomic gases. The system of balance equations adopted in the theory has the binary hierarchy structure

$$\frac{\partial F}{\partial t} + \frac{\partial F_k}{\partial x_k} = 0,$$
$$\frac{\partial F_i}{\partial t} + \frac{\partial F_{ik}}{\partial x_k} = 0,$$
$$\frac{\partial F_{ij}}{\partial t} + \frac{\partial F_{ijk}}{\partial x_k} = P_{ij}, \qquad \frac{\partial G_{ll}}{\partial t} + \frac{\partial G_{iik}}{\partial x_k} = 0,$$
$$\frac{\partial G_{lli}}{\partial t} + \frac{\partial G_{llik}}{\partial x_k} = Q_{lli}, \tag{6}$$

where G_{ll} is the energy density, G_{lli} is the energy flux, G_{llik} is the flux of G_{lli}, and Q_{lli} is the production of G_{lli}. The equations for the densities F, F_i and G_{ll} express the conservation laws of mass, momentum and energy, respectively. Therefore we have the relations

$$F = \rho, \qquad F_i = \rho v_i, \qquad F_{ij} = \rho v_i v_j - t_{ij},$$
$$G_{ll} = \rho v^2 + 2\rho\varepsilon, \qquad G_{lli} = \rho v^2 v_i - 2t_{il}v_l + 2q_i. \tag{7}$$

Now the number of the equations is 14 because there exists the dynamic pressure, which is absent in rarefied monatomic gases. This is the reason why the relations (5) are no more valid, and the trace of the momentum flux F_{ll} and the energy density G_{ll} play different roles to each other. By the method of closure in ET, we obtain the closed system of equations with the independent variables: ρ, v_i, ε, Π, $S_{\langle ij \rangle}$ and q_i.

The new 14-field theory is more appropriate than the previous works [9–14] because the constitutive equations are completely determined by the thermal and caloric equations of state together with the experimental data on the viscosities and the heat conductivity. Moreover the classical Navier–Stokes–Fourier model can be regarded as a particular model derived from this theory via the *Maxwellian iteration* [15]. The theory has also a firm mathematical background because the system is symmetric hyperbolic.

The new theory is now applied to rarefied polyatomic gases with the equations of state

$$p = \frac{k_B}{m}\rho T, \qquad \varepsilon = \frac{D}{2}\frac{p}{\rho} \quad (D = 3 + f) \tag{8}$$

where T, k_B and m are the temperature, the Boltzmann constant and the mass of a molecule, respectively. Here D is the degrees of freedom of a molecule given by the sum of the space dimension 3 for the translational motion and the internal degrees of freedom f ($\geqslant 0$). For monatomic gases, $D = 3$.

The system of balance equations for rarefied polyatomic gases with the thermal and caloric equations of state (8) is explicitly expressed as follows, where D is assumed to be constant [7]

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_k}{\partial x_k} = 0,$$

$$\rho\frac{\partial v_i}{\partial t} + \rho v_k\frac{\partial v_i}{\partial x_k} + \frac{\partial p}{\partial x_i} + \frac{\partial \Pi}{\partial x_i} - \frac{\partial S_{\langle ij \rangle}}{\partial x_j} = 0,$$

$$\frac{D}{2}\frac{k_B}{m}\rho\left(\frac{\partial T}{\partial t} + v_k\frac{\partial T}{\partial x_k}\right) + \frac{\partial q_k}{\partial x_k}$$
$$+ \left((p + \Pi)\delta_{ik} - S_{\langle ik \rangle}\right)\frac{\partial v_i}{\partial x_k} = 0,$$

$$\frac{\partial S_{\langle ij \rangle}}{\partial t} + v_k\frac{\partial S_{\langle ij \rangle}}{\partial x_k} - 2p\frac{\partial v_{\langle i}}{\partial x_{j \rangle}} + S_{\langle ij \rangle}\frac{\partial v_k}{\partial x_k} - 2\Pi\frac{\partial v_{\langle i}}{\partial x_{j \rangle}}$$
$$+ 2\frac{\partial v_{\langle i}}{\partial x_k}S_{\langle j \rangle k \rangle} - \frac{4}{D + 2}\frac{\partial q_{\langle i}}{\partial x_{j \rangle}} = -\frac{1}{\tau_S}S_{\langle ij \rangle},$$

$$\frac{\partial \Pi}{\partial t} + v_k\frac{\partial \Pi}{\partial x_k} + \frac{2(D - 3)}{3D}p\frac{\partial v_k}{\partial x_k} + \frac{5D - 6}{3D}\Pi\frac{\partial v_k}{\partial x_k}$$
$$- \frac{2(D - 3)}{3D}\frac{\partial v_{\langle i}}{\partial x_{k \rangle}}S_{\langle ik \rangle} + \frac{4(D - 3)}{3D(D + 2)}\frac{\partial q_k}{\partial x_k} = -\frac{1}{\tau_\Pi}\Pi,$$

$$\frac{\partial q_i}{\partial t} + v_k\frac{\partial q_i}{\partial x_k} + \frac{D + 4}{D + 2}q_i\frac{\partial v_k}{\partial x_k} + \frac{2}{D + 2}q_k\frac{\partial v_k}{\partial x_i}$$
$$+ \frac{D + 4}{D + 2}q_k\frac{\partial v_i}{\partial x_k} - \frac{k_B}{m}\frac{T}{\rho}(\Pi\delta_{ki} - S_{\langle ki \rangle})\frac{\partial \rho}{\partial x_k}$$
$$+ \frac{D + 2}{2}\frac{k_B}{m}\left((p + \Pi)\delta_{ki} - S_{\langle ki \rangle}\right)\frac{\partial T}{\partial x_k}$$
$$+ \frac{1}{\rho}\left((p - \Pi)\delta_{ki} + S_{\langle ki \rangle}\right)\left(\frac{\partial \Pi}{\partial x_k} - \frac{\partial S_{\langle kl \rangle}}{\partial x_l}\right) = -\frac{1}{\tau_q}q_i, \tag{9}$$

where the relaxation times τ_S, τ_Π and τ_q are positive functions of ρ and T.

The 14-field theory (9) was proved to be fully consistent with the kinetic theory using the method of MEP [16]. Moreover, from the studies of linear waves, the validity of the theory was confirmed by the consistency between the theoretical predictions and the experimental data [17].

The point that is not completely clarified in the theory until now is the limiting process from polyatomic to monatomic rarefied gases when we let D approach 3 from above, where D is assumed to be a continuous variable. The limit is singular in the sense that the system for rarefied polyatomic gases with 14 independent variables seems to converge to the system with only 13 independent variables for rarefied monatomic gases.

The singularity can be seen also by the inequalities required for the symmetric hyperbolicity in equilibrium. This requirement is always satisfied in the 13-field theory of monatomic gases, while, in the present 14-field theory, it is expressed by the inequality $D > 3$ [7]. The condition is obviously satisfied only for polyatomic gases with $D > 3$, and the case of monatomic gases with $D = 3$ is not admissible. Therefore only the limit of D toward 3 from above is meaningful.

The purpose of the present Letter is to clarify the singular limit. In Section 2, we will study the system of basic equations (9) in the limit $D \to 3$. We will see that a solution of (9) converges to the corresponding solution of (1) under the naturally conditioned ini-