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Monatomic gas as a singular limit of polyatomic gas in molecular extended thermodynamics with many moments

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HIGHLIGHTS

- Molecular extended thermodynamics of monatomic gas and of polyatomic gas are compared.
- Monatomic gas as a singular limit of polyatomic gas is studied.
- In the singular limit it is proved that the characteristic variables of polyatomic gas vanish.
- In one-dimensional case the constitutive equations of typical systems are derived.
- Asymptotic behaviors of linear wave and of shock wave in the singular limit are studied.

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ABSTRACT

The difference in the theoretical structure between monatomic and polyatomic gases in highly nonequilibrium states is discussed from the viewpoint of molecular extended thermodynamics (MET) of rarefied gases, which is free from the local equilibrium assumption. The MET theories of these two types of gases are based on the moment balance equations with different hierarchy structures due to whether the internal degrees of freedom of a molecule are incorporated in their distribution functions or not. In particular, the number of balance equations in the MET theory of polyatomic gases is greater than the number in the corresponding theory of monatomic gases. The closure procedure for the system of balance

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equations of polyatomic gases obtained in a recent paper (Arima et al., 2014) is adopted. We prove that the solutions for polyatomic gases converge, in the limit where the degrees of freedom of a molecule *D* tend to 3, to the ones for monatomic gases provided that we impose appropriate initial conditions compatible with monatomic gases. Thus a MET theory of rarefied monatomic gases can be identified as a singular limit of the corresponding MET theory of rarefied polyatomic gases. As illustrative examples, the asymptotic behaviors when $D \rightarrow 3$ in the dispersion relation of ultrasonic waves and in the shock wave structure are shown.

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1. Introduction

In a thermodynamic theory of rarefied gases composed of molecules, it is sometimes convenient to classify them into two groups, monatomic and polyatomic gases. A polyatomic molecule has both the translational degrees of freedom and the internal – rotational and vibrational – degrees of freedom, while a monatomic molecule has only the translational degrees of freedom. In an appropriate temperature range, we can assume that the translational degrees of freedom are fully excited and satisfy the equipartition law of energy, and also assume that some of the internal degrees of freedom, say rotational and vibrational degrees of freedom, are excited but the others are not. Total excited degrees of freedom will be referred to as *effective* degrees of freedom. We will confine our study within such a temperature range throughout the present paper. If the internal modes are totally frozen, a polyatomic gas behaves *monatomic like*.

There are characteristic quantities expressing the difference between monatomic and polyatomic gases. In the case of perfect fluids described by the Euler system of equations, the difference shows up only in the caloric equation of state (see (7)) through the effective degrees of freedom of a molecule *D*. As mentioned above, D = 3 for monatomic gases and D > 3 for polyatomic gases. For the description of viscous heat-conducting fluids, the Navier–Stokes–Fourier (NSF) theory [1,2] has frequently been adopted under the assumption of local equilibrium. In this case the caloric equation of state alone is not sufficient to distinguish monatomic and polyatomic gases, because the dynamic pressure (nonequilibrium pressure) Π associated with the bulk viscosity ν exists in polyatomic gases. Therefore polyatomic gases are characterized by D > 3, $\nu \neq 0$ and $\Pi \neq 0$, while the behavior of monatomic gases is described in the limit to D = 3, $\nu = 0$ and $\Pi = 0$ (the Stokes assumption).

Rational extended thermodynamics (RET, or simply ET) was proposed and developed to obtain hyperbolic systems, which, in the limit of small relaxation times, reduce to the parabolic system of NSF both in monatomic gases (13-field theory) [3] and polyatomic gases (14-field theory) [4]. The spirit of the RET theory is to close phenomenologically the system of balance equations with local-type constitutive equations by imposing the universal physical principles; *entropy*, *causality*, and *objectivity principles*. In principle this phenomenological approach can be done also when the number of field is large but there are technical mathematical difficulties.

To overcome these difficulties an alternative closure procedure was proposed. In this procedure, we assume that the independent variables are expressed in terms of the moments of a distribution function and according with the proposal of Müller and Ruggeri [5], we call the theory *molecular extended thermodynamics* (MET). In MET we can adopt the *maximum entropy principle* (MEP), which says that the most suitable distribution function maximizes the entropy density under some constraints. MEP was developed in [6,5] for monatomic gases and in [7,8] for polyatomic gases.

In the framework of MET, the equivalence between the closure procedures based on the entropy principle and on the MEP was proved by Boillat and Ruggeri [9] in the case of monatomic gases and recently by Arima, Mentrelli and Ruggeri [8,10] for polyatomic gases (see also [4]).

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