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Molecular extended thermodynamics: comparison between rarefied polyatomic and monatomic gas closures

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Abstract Molecular extended thermodynamics is justified at the mesoscopic level by the moment equations associated with the Boltzmann equation. For polyatomic gases we have a binary hierarchy of moments in contrast with the usual single hierarchy for monatomic gases. In this paper, taking one-dimensional space variables for simplicity, we review the closure of the system of the moment equations for polyatomic gases with the use of the maximum entropy principle, which is equivalent to the entropy principle. Then we consider the singular limit where the degrees of freedom of a molecule approach 3, and we prove that, by imposing appropriate initial conditions, the solutions for polyatomic gases converge to the ones for monatomic gases. As examples of the singular limit, the asymptotic behaviors of linear waves and light scattering based on the linearized system of field equations are briefly presented.

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1 Introduction

In order to capture a highly nonequilibrium phenomena in rarefied monatomic gases such as the sound wave in high-frequency region and the shock wave with large Mach number, the molecular extended thermodynamics (MET) which describes a state of a gas by the moments of a distribution function has been proposed [1–3]. The closure of MET is achieved by the maximum entropy principle: the most suitable distribution function maximizes the entropy density under some constraints, which is equivalent to the entropy principle [4]. Since this theory is based on the Boltzmann equation, the system of the moment equations has a *single* tensorial hierarchy starting from the conservation laws of mass, momentum and energy, in which the flux in one equation becomes the density in the next equation. MET is compatible with the phenomenological approach which adopts the system of balance equations with local-type constitutive equations satisfying the entropy, causality, and objectivity principles, such as the 13-field theory that adopts the mass density, the velocity, the specific internal energy, the shear stress and the heat flux as independent fields [5].

For rarefied polyatomic gases the MET theory has been proposed [6–9] based on the kinetic model by Bourgat et al. [10] in which the distribution function depends on an additional continuous variable representing the internal energy of a molecule. In contrast with MET for monatomic gases, the system of moment equations has a *binary* hierarchy; one hierarchy starts from the balance equations for mass density, momentum density and momentum flux, and the other one starts from the balance equations for energy density and energy flux. This theory is in agreement with the phenomenological 14-field theory that adopts the dynamic (nonequilibrium) pressure in addition to the 13 fields [11–13] and has been successful to explain various phenomena [14–20].

The difference of the hierarchy of moment equations between the MET theories for rarefied monatomic gases and for rarefied polyatomic gases is due to the existence of the nonequilibrium variables that characterize polyatomic gases. In the case of the 14-field theory for polyatomic gases, the dynamic pressure plays a role of such characteristic variables. In the limit, so-called singular limit, that the degrees of freedom D approach 3 under an appropriate initial condition compatible with a property of monatomic gases, i.e., the dynamic pressure vanishes, the binary hierarchy of the 14-field theory converges to the single hierarchy of the monatomic 13-field theory, and the dynamic pressure vanishes at any time [21]. In a general case with many independent fields, there emerge many characteristic variables. Recently, in such a case, we proved that the ET theory of monatomic gases is also derived as a singular limit of the theory of polyatomic gases, and the characteristic variables of polyatomic gases vanish at any time [22].

In the present paper, we briefly summarize the singular limit of MET for rarefied polyatomic gases to the one for monatomic gases. And examples of the asymptotic behavior of the solution in the limit are shown in the cases of linear waves and light scattering. Another example was discussed in [22].

2 Molecular extended thermodynamics for rarefied polyatomic gases in one-dimensional case

A rarefied polyatomic gas in equilibrium is characterized by the equations of state:

$$p = \frac{k_B}{m}\rho T, \quad \varepsilon = \frac{D}{2}\frac{k_B}{m}T, \tag{1}$$

where p, ε, ρ, T, D, k_B, m are, respectively, the pressure, specific internal energy, mass density, temperature, degrees of freedom of a molecule, Boltzmann constant and mass of a molecule. In a temperature range where the translational degrees of freedom are fully excited and the equipartition law of energy is satisfied, the degrees of freedom satisfy $D > 3$ since the internal degrees of freedom, that is, the rotational and vibrational degrees of freedom, are excited. In the present study, we assume that other internal degrees of freedom are not excited.

From a kinetic theoretical viewpoint, the model for a polyatomic gas is proposed by Bourgat et al. [10] in the framework of the Borgnakke–Larsen procedure [23]. The basic feature of the model is the presence of a non-negative parameter I that reflects the internal degrees of freedom of a molecule. The model is prescribed by the one-body distribution function $f(\mathbf{x}, \mathbf{c}, t, I)$, where $\mathbf{x}$, $\mathbf{c}$, t and I are, respectively, the position, the velocity of a molecule, the time and the specific internal energy of a molecule. The rate of change of the distribution function in the absence of external force is determined by the Boltzmann like equation:

$$\partial_t f + c_i\, \partial_i f = Q(f), \tag{2}$$

where the symbols ∂_t and ∂_i denote partial derivatives with respect to t and x_i ($i = 1, 2, 3$).[1] The collision term $Q(f)$ in the right-hand side of (2) also takes into account the influence of the internal degrees of freedom through the collisional cross section.

2.1 Balance equations and velocity independent fields

Let us study a one-dimensional problem along the $x(\equiv x_1)$-axis. In the MET theory, the evolution of a nonequilibrium state of a gas is described by the following balance equations obtained from (2):

[1] Throughout the paper, summation with respect to repeated indexes is assumed, where the range of the sum is to be understood in the context: when the index represents a spatial coordinate, the range of the sum is from 1 to 3; in all the other cases the sum is intended over the variability region of the repeated indexes.

$$\partial_t F_{p,q} + \partial_x F_{p+1,q} = P_{p,q}, \qquad \partial_t G_{p',q'} + \partial_x G_{p'+1,q'} = Q_{p',q'}, \tag{3}$$

where ∂_x denotes the partial derivative with respect to x, and the indexes are the non-negative integers satisfying

$$0 \leqslant p + 2q \leqslant N, \quad 0 \leqslant p' + 2q' \leqslant M.$$

The system (3) is denoted as "(N, M)-system". The moments are defined as follows:

$$F_{p,q} = \int_{\mathbb{R}^3} \int_0^\infty mf\,(c_1)^p \left(c^2\right)^q I^\delta\, dI d\mathbf{c},$$
$$G_{p',q'} = \int_{\mathbb{R}^3} \int_0^\infty mf \left(c^2 + \frac{2I}{m}\right) (c_1)^{p'} \left(c^2\right)^{q'} I^\delta\, dI d\mathbf{c},$$

and the production terms $P_{p,q}$ and $Q_{p',q'}$ are defined in a similar way as follows:

$$P_{p,q} = \int_{\mathbb{R}^3} \int_0^\infty mQ(f)(c_1)^p \left(c^2\right)^q I^\delta\, dI d\mathbf{c},$$
$$Q_{p',q'} = \int_{\mathbb{R}^3} \int_0^\infty mQ(f) \left(c^2 + \frac{2I}{m}\right) (c_1)^{p'} \left(c^2\right)^{q'} I^\delta\, dI d\mathbf{c},$$

where $c^2 = c_i c_i$ and $\delta = (D-5)/2$ ($\delta > -1$) so as to recover the caloric equation of state for polyatomic gases in equilibrium $(1)_2$.

It is worth noting that the first two equations of the F-hierarchy represent the conservation laws of mass and momentum, the first equation of the G-hierarchy represents the conservation law of energy. Therefore the first 14 fields are identified as the macroscopic variables commonly used:

$$F_{0,0} = \rho, \quad F_{1,0} = \rho v, \quad F_{2,0} = p + \Pi - \sigma + \rho v^2, \quad F_{0,1} = 3(p + \Pi) + \rho v^2,$$
$$G_{0,0} = 2\rho\varepsilon + \rho v^2, \quad G_{1,0} = 2q + 2(\rho\varepsilon + p + \Pi - \sigma)v + \rho v^3, \tag{4}$$

where v, q, Π, and σ being, respectively, the velocity, the heat flux, the dynamic pressure and the shear stress.

In [8], it was proved that the requirement of the Galilean invariance of the system implies $M \leqslant N - 1$. This requirement and one more requirement that equilibrium characteristic velocities depend on the degrees of freedom D bring us to the conclusion: $M = N - 1$. The Euler system ((1, 0)-system) with 5 moments: $F_{0,0}$, $F_{1,0}$, $G_{0,0}$, and the ET theory with 14 moments: $F_{0,0}$, $F_{1,0}$, $F_{2,0}$, $F_{0,1}$, $G_{0,0}$, $G_{1,0}$ ((2, 1)-system) are typical examples of this case. In the present and next section, we concentrate on the study of the $(N, N-1)$-system.

By adopting the peculiar velocity $C_1 = c_1 - v$ instead of the velocity of a molecule c_1, the moments are expressed in terms of the velocity independent variables as follows:

$$F_{p,q} = \sum_{r=0}^{N} \sum_{s=0}^{[r/2]} X_{p,q,r-2s,s} \hat{F}_{r-2s,s},$$

$$G_{p',q'} = \sum_{r'=0}^{N-1} \sum_{s'=0}^{[r'/2]} X_{p',q',r'-2s',s'} \left(\hat{G}_{r'-2s',s'} + 2v \hat{F}_{r'-2s'+1,s'} + v^2 \hat{F}_{r'-2s',s'} \right),$$

where variables with a hat are the velocity independent variables. The coefficients are defined as follows:

$$X_{p,q,r,s} = \begin{cases} \displaystyle\sum_{j=\max(0,q-r-s)}^{\min(p+q-r-s,q-s)} \binom{p}{p+q-r-s-j} \binom{q}{q-s} \binom{q-s}{j} 2^{q-s-j} v^{p+2q-(r+2s)} & \text{if } q \geqslant s \text{ and } p+q \geqslant r+s \\ 0 & \text{otherwise} \end{cases}. \tag{5}$$

2.2 Closure by means of MET near equilibrium

In equilibrium, the distribution function f^E is obtained by Pavić, Ruggeri and Simić [7] (see also [24]) as follows:

$$f^E = \frac{1}{A(T)} \frac{\rho}{m} \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp\left(-\frac{m}{2k_B T} \left(C^2 + \frac{2I}{m} \right) \right).$$

The normalization function $A(T)$ is given by

$$A(T) = \int_0^\infty \exp\left(-\frac{I}{k_B T} \right) I^\delta \, dI = (k_B T)^{1+\delta} \Gamma(1+\delta),$$

where Γ denotes the gamma function.

Near equilibrium, the distribution function f is expanded around f^E. Then the constitutive equations for fluxes are obtained explicitly by means of MET [1,6]. For simplicity, let us introduce a vector $\hat{\boldsymbol{U}}$ that denotes a set of velocity independent part of densities and a vector $\hat{\boldsymbol{U}}^1$ that denotes a set of velocity independent part of fluxes:

$$\hat{\boldsymbol{U}} = \begin{pmatrix} \hat{F}_{p,q} \\ \hat{G}_{p',q'} \end{pmatrix}, \quad \hat{\boldsymbol{U}}^1 = \begin{pmatrix} \hat{F}_{p+1,q} \\ \hat{G}_{p'+1,q'} \end{pmatrix}.$$

As the result of the closure, the fluxes are expressed by the densities as follows:

$$\tilde{\hat{\boldsymbol{U}}}^1 = \hat{\boldsymbol{J}}^1 \left(\hat{\boldsymbol{J}} \right)^{-1} \tilde{\hat{\boldsymbol{U}}}, \quad \tilde{\hat{\boldsymbol{U}}} = \hat{\boldsymbol{U}} - \hat{\boldsymbol{U}}^E, \quad \tilde{\hat{\boldsymbol{U}}}^1 = \hat{\boldsymbol{U}}^1 - \left(\hat{\boldsymbol{U}}^1 \right)^E, \tag{6}$$

where the superscript "E" means that a quantity is evaluated in a local equilibrium state and therefore a quantity with a tilde indicates the nonequilibrium part. The coefficient matrices are defined as follows [8]:

$$\hat{\boldsymbol{J}} = \begin{pmatrix} \hat{J}^{\mathcal{M}}_{p+r,q+s} & \hat{J}^{1|E}_{p+r',q+s'} \\ \hat{J}^{1|E}_{p'+r,q'+s} & \hat{J}^{2|E}_{p'+r',q'+s'} \end{pmatrix}, \qquad \hat{\boldsymbol{J}}^1 = \begin{pmatrix} \hat{J}^{\mathcal{M}}_{p+r+1,q+s} & \hat{J}^{1|E}_{p+r'+1,q+s'} \\ \hat{J}^{1|E}_{p'+r+1,q'+s} & \hat{J}^{2|E}_{p'+r'+1,q'+s'} \end{pmatrix},$$

where the elements are given by

$$\begin{aligned} \hat{J}^{\mathcal{M}}_{p,q} =& -\frac{m}{k_B}\rho\left(\frac{k_BT}{m}\right)^{\frac{p}{2}+q}\frac{2^{\frac{p}{2}+q}}{p+1}\Gamma\left(\frac{p+3}{2}+q\right)\frac{1+(-1)^p}{\sqrt{\pi}}, \\ \hat{J}^{1|E}_{p,q} =& \hat{J}^{\mathcal{M}}_{p,q+1} + 2\frac{k_B}{m}T(1+\delta)\hat{J}^{\mathcal{M}}_{p,q}, \\ \hat{J}^{2|E}_{p,q} =& \hat{J}^{\mathcal{M}}_{p,q+2} + 4\frac{k_B}{m}T(1+\delta)(2+\delta)\left(\hat{J}^{\mathcal{M}}_{p,q+1} + \frac{k_B}{m}T(2+\delta)\hat{J}^{\mathcal{M}}_{p,q}\right). \end{aligned}$$

3 Singular limit of polyatomic gases to monatomic gases

In [22], it was shown that the nonequilibrium parts of the difference between F and G-series play a role of the characteristic nonequilibrium variables of polyatomic gases:

$$\hat{\Pi}_{p'',q''} = \tilde{\hat{F}}_{p'',q''+1} - \tilde{\hat{G}}_{p'',q''}, \quad (0 \leqslant p'' + 2q'' \leqslant N-2).$$

The dynamic pressure Π is the first component of $\hat{\Pi}_{p'',q''}$ except for the factor $1/3$. We call these multi-index tensors $\hat{\Pi}_{p'',q''}$ *the dynamical multi-index pressure tensors*.

The evolution of the dynamic pressure tensors can be studied by taking $\{\hat{F}_{p,0}, \hat{G}_{p',q'}, \hat{\Pi}_{p'',q''}, v\}\}$ as independent variables instead of $\{\hat{F}_{p,q}, \hat{G}_{p',q'}, v\}$. In the limit of $D \to 3$ ($\delta \to -1$) where D is assumed to be a continuous variable, it is proved that the field equations of $\hat{\Pi}_{p'',q''}$ with closed fluxes (6) are the first-order quasi-linear partial differential equations with respect to $\hat{\Pi}_{p'',q''}$. Imposing the initial condition compatible with a property of monatomic gases, i.e.,

$$\hat{\Pi}_{p'',q''}(\boldsymbol{x}, 0) = 0,$$

and assuming the uniqueness of the solution of $\hat{\Pi}_{p'',q''}$, we obtain

$$\hat{\Pi}_{p'',q''}(\boldsymbol{x}, t) = 0, \qquad \forall t.$$

It is also proved that the balance equations of non-vanishing fields $\{F_{p,0}, G_{p',q'}\}$ have the same hierarchy structure as that of monatomic gases. In the singular limit, since we have

$$\lim_{D\to 3} G_{p',q'} = \lim_{D\to 3} F_{p',q'+1},$$

the system of field equations of $\{\lim_{D\to 3} F_{p,0}, \lim_{D\to 3} G_{p',q'}\}$ can be rewritten as follows:

$$\partial_t \left(\lim_{D\to 3} F_{p,q} \right) + \partial_i \left(\lim_{D\to 3} F_{p+1,q} \right) = \lim_{D\to 3} P_{p,q},$$
$$\partial_t \left(\lim_{D\to 3} F_{p^*,q^*+1} \right) + \partial_i \left(\lim_{D\to 3} F_{p^*+1,q^*+1} \right) = \lim_{D\to 3} P_{p^*,q^*+1},$$

where the non-negative integers satisfy $p^* + 2q^* = N - 1$. This system of balance equations, called $((N+1)^-)$-system, has a single hierarchy. The (3^-)-system with 13 moments; $F_{0,0}$, $F_{1,0}$, $F_{2,0}$, $F_{0,1}$, $F_{1,1}$ is a particular example.

To sum up, in the singular limit, the dynamical pressure tensors vanish and the polyatomic $(N, N-1)$-system with binary hierarchy structure coincides with the monatomic $((N+1)^-)$-system with single hierarchy structure.

Similar to this result it is also proved that $((N+1)^-, M)$-system with $M \leq N-1$ of which characteristic velocities do not depend on D also converges to $((N+1)^-)$-system. One of the examples is the ET theory with 6 moments; $F_{0,0}$, $F_{1,0}$, $F_{0,1}$, $G_{0,0}$, $((2^-, 0)$-system) [25–27]. This theory is the simplest theory next to the Euler system, and recently the theory with nonlinear constitutive equations was proposed and developed [28–32]. In the singular limit, the $(2^-, 0)$-system converges to the Euler system for monatomic gases $((2^-)$-system) [21]. The ET theory with 17 moments; $F_{0,0}$, $F_{1,0}$, $F_{2,0}$, $F_{0,1}$, $F_{1,1}$, $G_{0,0}$, $G_{1,0}$, $((3^-, 1)$-system) is another example. This theory is in full agreement with the kinetic theory of polyatomic gases [33] that introduces an internal mode of the energy and the internal heat flux. In the singular limit, the $(3^-, 1)$-system converges to the (3^-)-system.

4 Examples of the convergence of the solutions in the singular limit

Let us study the asymptotic behaviors in the dispersion relation of sound waves and the dynamic structure factor in light scattering when D approaches 3. See also [22]. As particular examples, we consider the convergence of the $(2, 1)$ and $(3^-, 1)$-systems to (3^-)-system, and of the $(3, 2)$ and $(4^-, 2)$-systems to (4^-)-system. As seen in (4), the dynamical pressure tensor of $(2, 1)$-system is only the dynamic pressure Π. For $(3^-, 1)$ and $(3, 2)$-systems and $(4^-, 2)$-system, the dynamical pressure tensors are, respectively, Π and $\hat{\Pi}_{1,0}$, and Π, $\hat{\Pi}_{1,0}$ and $\hat{\Pi}_{2,0}$.

In the present analysis, we adopt, as simplest example, the BGK-model which close the production terms by the densities as follows:

$$P_{p,q} = -\frac{1}{\tau}\tilde{F}_{p,q}, \quad Q_{p',q'} = -\frac{1}{\tau}\tilde{G}_{p',q'},$$

where τ denotes the relaxation time.

4.1 Linearized system

Usually we are interested in the time evolution of the nonequilibrium part of the fields in addition to the hydrodynamic variables ρ, v and ε. Therefore we adopt the following variables as independent fields:

$$\hat{\boldsymbol{u}} = \left(\rho,\ v,\ \tilde{\hat{F}}_{0,1},\ \tilde{\hat{F}}_{2,0},\ \ldots,\ \tilde{\hat{F}}_{p,q},\ \varepsilon,\ \tilde{\hat{G}}_{1,0},\ \ldots,\ \tilde{\hat{G}}_{p',q'}\right)^T.$$

Let $\hat{\boldsymbol{u}}_0$ be a constant equilibrium state, then the linearized system for the perturbed field $\bar{\boldsymbol{u}}$ around $\hat{\boldsymbol{u}}_0$ ($\hat{\boldsymbol{u}} = \hat{\boldsymbol{u}}_0 + \bar{\boldsymbol{u}}$) is written as follows:

$$H^0_{ij}\partial_t \bar{u}_j + H^1_{ij}\partial_x \bar{u}_j = H^P_{ij}\bar{u}_j. \tag{7}$$

The coefficients are defined by

$$H^0_{ij} = \begin{cases} \left(B_{ik}\hat{U}_k\right)_0 & \text{if } \bar{u}_j = \bar{v} \\ \left(\frac{\partial \hat{U}_i}{\partial \bar{u}_j}\right)_0 & \text{otherwise} \end{cases}, \qquad H^1_{ij} = \begin{cases} \left(\hat{U}_i + B_{ik}\hat{U}^1_k\right)_0 & \text{if } \bar{u}_j = \bar{v} \\ \left(\frac{\partial \hat{U}^1_i}{\partial \bar{u}_j}\right)_0 & \text{otherwise} \end{cases},$$

$$H^P_{ij} = \begin{cases} 0 & \text{if } \bar{u}_j = \bar{\rho}, \bar{v}, \bar{\varepsilon} \\ -\frac{1}{\tau}\delta_{ij} & \text{otherwise} \end{cases},$$

where the subscript "0" indicates a quantity evaluated at the reference equilibrium state, and B_{ik} is an element of the following matrix:

$$\boldsymbol{B} = \begin{pmatrix} A_{p,q,r,s} & 0 \\ 2\delta_{p'+1,r}\delta_{q',s} & A_{p',q',r',s'} \end{pmatrix}.$$

The element $A_{p,q,r,s}$ is determined by (5) [1,34] as follows:

$$A_{p,q,r,s} = \begin{cases} \sum_{j=\max(0,q-r-s)}^{\min(p+q-r-s,q-s)} \binom{p}{p+q-r-s-j}\binom{q}{q-s}\binom{q-s}{j}(p+2q-(r+2s))\,2^{q-s-j}\delta_{p+2q,r+2s+1} & \text{if } q \geqslant s \text{ and } p+q \geqslant r+s \\ 0 & \text{otherwise} \end{cases}.$$

4.2 Dispersion relation of sound wave in the singular limit

We study one-dimensional linear harmonic waves with the wave form:

$$\bar{\boldsymbol{u}} = \bar{\boldsymbol{u}}^{Amp} \mathrm{e}^{\mathrm{i}(\omega t - kx)}, \tag{8}$$

where $\bar{\boldsymbol{u}}^{Amp}$ is the constant amplitude vector, ω is the frequency, and k is the complex wave number. In [22], the asymptotic behaviors of the phase velocity and the attenuation factor are studied. Hereafter, we study the attenuation per wavelength α_λ because this qunaitity is important in experiments and is discussed in the context of ET [15].

By inserting the waveform (8) into the linearized system of field equations (7), we obtain the dispersion relation [14,35,36], from which α_λ is derived as the function of ω:

$$\alpha_\lambda(\omega) = -2\pi\frac{\Im(k)}{\Re(k)}.$$

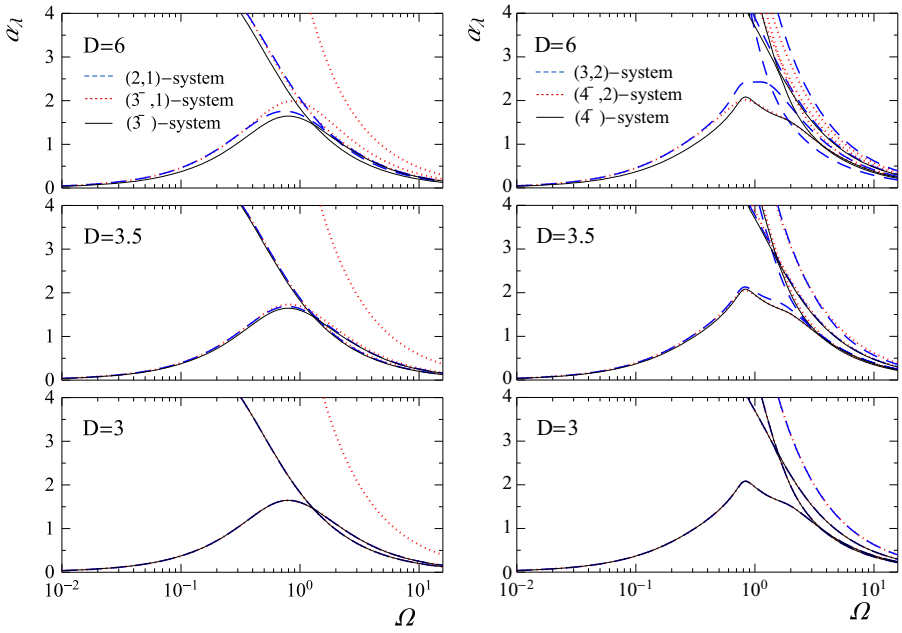

Fig. 1 Dependence of the attenuation per wavelength of $(2,1)$, $(3^-,1)$ and (3^-)-systems (*left*) and of $(3,2)$, $(4^-,2)$ and (4^-)-systems (*right*) on the dimensionless frequency for $D = 6,\ 3.5,\ 3$. The *solid lines* denote the monatomic (3^-) and (4^-)-systems. The *dashed lines* denote the polyatomic $(2,1)$ and $(3,2)$-systems. The *dotted lines* denote the polyatomic $(3^-,1)$ and $(4^-,2)$-systems

In Fig. 1, we show the dependence of α_λ with $D = 6,\ 3.5,\ 3$ on the reduced frequency $\Omega\ (= \tau\omega)$ in the $(2,1)$, $(3^-,1)$, $(3,2)$ and $(4^-,2)$-systems. When $D \to 3$, the dispersion relations of both $(2,1)$ and $(3^-,1)$-systems approach uniformly the dispersion relation of (3^-)-system of monatomic gases. We notice that a mode of $(3^-,1)$-system that comes from the system of the field equations of the dynamical pressure tensors has no counterpart in ET of monatomic gases. Since the solutions of such variables are zero in $D \to 3$ because of the initial condition, the amplitude of this mode is zero. Similarly, the dispersion relations of both $(3,2)$ and $(4^-,2)$-systems approach uniformly the dispersion relation of (4^-)-system of monatomic gases.

4.3 Light scattering

We analyze the asymptotic behavior of light scattering. The light scattering occurs due to the fluctuations in the mass density ρ through the dielectric constant $\epsilon(\rho)$, and the intensity of scattered light is directly related to the dynamic structure factor [1,6]:

$$S(\boldsymbol{q},\omega) = \frac{1}{\pi}\left(\frac{\partial\epsilon}{\partial\rho}\right)^2 \Re\langle\delta\rho^*(\boldsymbol{q},0)\delta\hat{\rho}(\boldsymbol{q},s)\rangle_{s=i\omega}.$$

where $\boldsymbol{q}$ is the scattering vector, magnitude of which is $q = (4\pi/\Lambda)\sin(\theta/2)$ with Λ and θ being the wavelength of the incident light and the scattering angle, ω is the

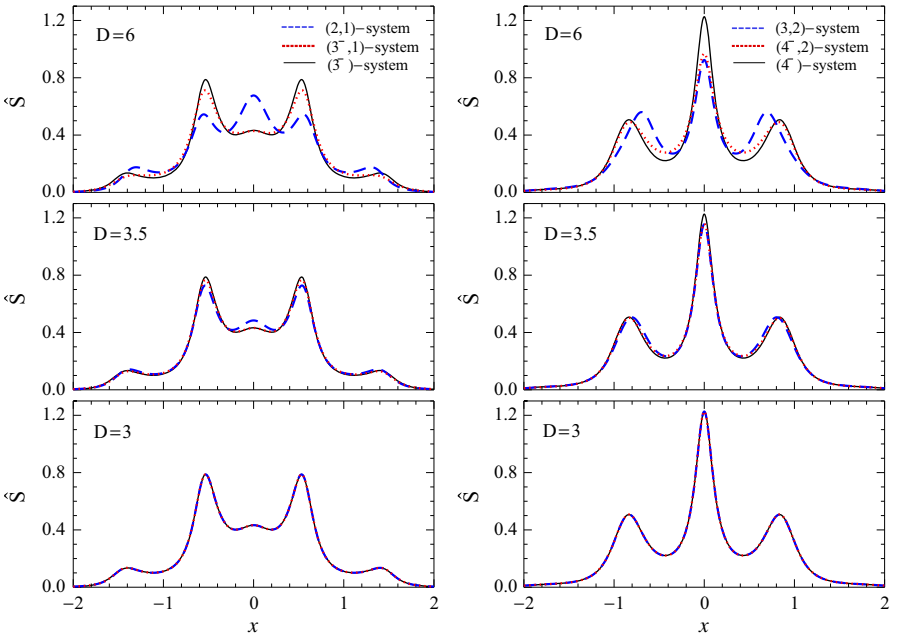

Fig. 2 The relative intensity of the dynamic structure factor of (2, 1), $(3^-, 1)$ and (3^-)-systems (*left*) and of (3, 2), $(4^-, 2)$ and (4^-)-systems (*right*) for $D = 6, 3.5, 3$. The *solid lines* denote the monatomic (3^-) and (4^-)-systems. The *dashed lines* denote the polyatomic (2, 1) and (3, 2)-systems. The *dotted lines* denote the polyatomic $(3^-, 1)$ and $(4^-, 2)$-systems

shift in angular frequency, and $\langle \delta\rho^*(\boldsymbol{q}, 0)\delta\hat{\rho}(\boldsymbol{q}, s)\rangle$ is the Laplace transform of the autocorrelation of the density fluctuations $\langle \delta\rho^*(\boldsymbol{q}, 0)\delta\rho(\boldsymbol{q}, t)\rangle$ where $\langle\ \rangle$ denotes the thermal average and $\delta\rho(\boldsymbol{q}, t)$ is the Fourier transform of the mass density fluctuation $\delta\rho(\boldsymbol{x}, t)$.

It is useful to introduce the following dimensionless quantities:

$$x = \frac{\omega}{v_0 q}, \quad y = \frac{1}{\tau v_0 q},$$

where $v_0 = \sqrt{2k_B T_0/m}$. The relative intensity of $S(\boldsymbol{q}, \omega)$ can be expressed as a function of x, y, D. Usually the case of large y is referred to as the hydrodynamic region and the case of small y as the kinetic region. In particular, in the kinetic region, the superiority of ET comparing to NSF becomes notable [1,18]. Therefore we study the asymptotic behavior in such region.

In Fig. 2 the dependences of the relative intensity of the dynamic structure factor $\hat{S}(x, y)$ on x with $y = 0.5$ are shown for $D = 6,\ 3.5,\ 3$. We define $\hat{S}(x, y)$ as follows:

$$\hat{S}(x,y) = \frac{S(x,y)}{\int_{x=-\infty}^{x=\infty} S(x,y)\mathrm{d}x} = \frac{\Re\left(\left(\frac{x}{\tau y}\boldsymbol{I} + \mathrm{i}\frac{1}{v_0\tau y}\left(\boldsymbol{H}^0\right)^{-1}\boldsymbol{H}^1 - \left(\boldsymbol{H}^0\right)^{-1}\boldsymbol{H}^P\right)^{-1}\right)_{11}}{\int_{x=-\infty}^{x=\infty}\Re\left(\left(\frac{x}{\tau y}\boldsymbol{I} + \mathrm{i}\frac{1}{v_0\tau y}\left(\boldsymbol{H}^0\right)^{-1}\boldsymbol{H}^1 - \left(\boldsymbol{H}^0\right)^{-1}\boldsymbol{H}^P\right)^{-1}\right)_{11}\mathrm{d}x},$$

where $\boldsymbol{I}$ is an identity matrix. We notice that the profiles of $\hat{S}(x, y)$ of $(2, 1)$ and $(3^-, 1)$-systems and of $(3, 2)$ and $(4, 2^-)$-systems, respectively, approach uniformly the corresponding profiles of monatomic gases in the singular limit.

5 Summary and concluding remarks

We have briefly summarized the singular limit of MET for polyatomic gases to the one for monatomic gas, that is, the convergence of the $(N, N-1)$-system with binary hierarchy to the $((N+1)^-)$-system with single hierarchy. Basing on this result we have shown the asymptotic behaviors of attenuation per wavelength of sound wave and of the dynamic structure factor. From these behaviors the role of the dynamical pressure tensors has been shown explicitly.

We make the following two remarks:

(i) The results exhibited in the present paper are also true for other systems [22]. In particular, (N)-system that is usually studied in the context of ET is derived as the singular limit of (N, M)-system with $M < N - 1$ where equilibrium characteristic velocities do not depend on D. In other words, the physically relevant system for monatomic gases is (N^-)-system instead of (N)-system.

(ii) In the present study, we adopt the BGK model. However, in practical problems, there exist several kinds of the relaxation times and the difference of the order of magnitude between the relaxation times plays an important role [37].

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