

Dispersion Relation for Sound in Rarefied Polyatomic Gases Based on Extended Thermodynamics

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Abstract We study the dispersion relation for sound in rarefied polyatomic gases (hydrogen, deuterium and hydrogen deuteride gases) basing on the recently developed theory of extended thermodynamics (ET) of dense gases. We compare the relation with those obtained in experiments and by the classical Navier-Stokes Fourier (NSF) theory. The applicable frequency-range of the ET theory is proved to be much wider than that of the NSF theory. We evaluate the values of the bulk viscosity and the relaxation times involved in nonequilibrium processes. The relaxation time related to the dynamic pressure has a possibility to become much larger than the other relaxation times related to the shear stress and the heat flux.

Keywords Extended thermodynamics · Rarefied polyatomic gases · Dispersion relation for sound · Phase velocity and absorption · Bulk viscosity · Relaxation time

1 Introduction

For extended thermodynamics (ET) of rarefied monatomic gases, there has been a well-established theory [1] for many years. In contrast, a corresponding ET theory for dense gases has been developed successfully only very recently [2] after several

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pioneering endeavors [3–8]. This is the theory of 14 fields of mass density, velocity, temperature, viscous stress, dynamic pressure, and heat flux with two parallel hierarchical series of field equations of balance type. The constitutive equations are determined explicitly by the thermal and caloric equations of state. The theory includes naturally the theory of *rarefied polyatomic* gases as a special case, and, in this case, it was proved recently that the theory is perfectly consistent with the kinetic theory [9]. Owing to the establishment of the theory for dense gases, the applicable range of ET has been enlarged enormously.

The purpose of the present paper is to understand explicitly the validity and the features of the new theory through studying the dispersion relation for sound. We firstly derive the dispersion relation, and secondly compare the results with those obtained in experiments and by the classical Navier-Stokes Fourier (NSF) theory based on the local equilibrium assumption [10, 11]. We will, however, confine our analysis within the sound in some rarefied diatomic gases because suitable experimental data are scarce and are mainly restricted to rarefied gases. The study of the dispersion relation for sound in general dense gases with and without internal degrees of freedom is, therefore, remained to be a future work.

The organization of the present paper is as follows: In Sec. 2, we summarize the basic equations necessary for the present analysis. In Sec. 3, the dispersion relation is derived and its high-frequency limit is studied. In Sec. 4, the dispersion relations in hydrogen, deuterium and hydrogen deuteride gases are compared with both experimental data and those derived from the NSF theory. We also evaluate the relaxation times and the bulk viscosity. The last section is devoted to the summary and concluding remarks.

2 Basic equations

In this section, we summarize the basic equations for the present analysis. We adopt the thermal and caloric equations of state for a classical (i.e., non-degenerate) ideal gas given by

$$p = a\rho T \quad \text{and} \quad \varepsilon = \varepsilon(T), \quad (1)$$

where p , ρ , T and ε are the pressure, mass density, absolute temperature and specific internal energy, respectively, and $a \equiv k_B/m$ with k_B and m being the Boltzmann constant and the mass of a molecule. Note that gases are, in general, non-polytropic, that is, the specific heat at constant volume

$$c_v = \frac{d\varepsilon}{dT} \quad (2)$$

is, in general, not constant but depends on the temperature.

We assume that a nonequilibrium state can be characterized by the 14 independent field variables $\mathbf{u} \equiv (\rho, v_i, T, S_{\langle ij \rangle}, \Pi, q_i)$ where v_i , $S_{\langle ij \rangle}$, $\Pi (= -S_{ii}/3)$ and q_i are, respectively, the velocity, symmetric traceless part of the viscous stress, dynamic pressure and heat flux [2]. Let $\mathbf{u}_0 \equiv (\rho_0, 0, T_0, 0, 0, 0)$ be a constant equilibrium state, then the linearized system in the neighborhood of \mathbf{u}_0 for the perturbed

field \mathbf{u} reads:

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \rho_0 \frac{\partial v_k}{\partial x_k} &= 0, \\
\rho_0 \frac{\partial v_i}{\partial t} + aT_0 \frac{\partial \rho}{\partial x_i} + a\rho_0 \frac{\partial T}{\partial x_i} - \frac{\partial S_{\langle ij \rangle}}{\partial x_j} + \frac{\partial \Pi}{\partial x_i} &= 0, \\
a\rho_0 c_v^* \frac{\partial T}{\partial t} + a\rho_0 T_0 \frac{\partial v_k}{\partial x_k} + \frac{\partial q_k}{\partial x_k} &= 0, \\
\frac{\partial S_{\langle ij \rangle}}{\partial t} - 2a\rho_0 T_0 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} - \frac{2}{1+c_v^*} \frac{\partial q_{\langle i}}{\partial x_{j \rangle}} &= -\frac{1}{\tau_S} S_{\langle ij \rangle}, \\
\frac{\partial \Pi}{\partial t} + \left(\frac{2}{3} - \frac{1}{c_v^*} \right) a\rho_0 T_0 \frac{\partial v_k}{\partial x_k} + \frac{2c_v^* - 3}{3c_v^*(1+c_v^*)} \frac{\partial q_k}{\partial x_k} &= -\frac{1}{\tau_\Pi} \Pi, \\
\frac{\partial q_i}{\partial t} + (1+c_v^*) a^2 \rho_0 T_0 \frac{\partial T}{\partial x_i} - aT_0 \frac{\partial S_{\langle ik \rangle}}{\partial x_k} + aT_0 \frac{\partial \Pi}{\partial x_i} &= -\frac{1}{\tau_q} q_i,
\end{aligned} \tag{3}$$

where c_v^* is the dimensionless specific heat at the reference equilibrium state:

$$c_v^* = \frac{c_{v0}}{a}. \tag{4}$$

The relaxation times τ_S, τ_Π and τ_q in Eq. (3) are also evaluated at the reference equilibrium state.

By the Maxwellian iteration [1, 2, 12], we obtain the relations between the relaxation times and the shear viscosity μ , bulk viscosity ν and heat conductivity κ :

$$\mu = a\rho_0 T_0 \tau_S, \quad \nu = \left(\frac{2}{3} - \frac{1}{c_v^*} \right) a\rho_0 T_0 \tau_\Pi, \quad \kappa = (1+c_v^*) a^2 \rho_0 T_0 \tau_q. \tag{5}$$

Let us consider a one-dimensional problem and assume:

$$v_i \equiv \begin{pmatrix} v \\ 0 \\ 0 \end{pmatrix}, \quad S_{\langle ij \rangle} \equiv \begin{pmatrix} S & 0 & 0 \\ 0 & -\frac{1}{2}S & 0 \\ 0 & 0 & -\frac{1}{2}S \end{pmatrix}, \quad q_i \equiv \begin{pmatrix} q \\ 0 \\ 0 \end{pmatrix}. \tag{6}$$

Then, from Eq. (3), the linearized basic field equations are neatly written as

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{A}_0 \frac{\partial \mathbf{u}}{\partial x} = \mathbf{B}_0 \mathbf{u}, \tag{7}$$

where \mathbf{A}_0 and \mathbf{B}_0 are given by

$$\mathbf{A}_0 = \begin{pmatrix} 0 & \rho_0 & 0 & 0 & 0 & 0 \\ \frac{aT_0}{\rho_0} & 0 & a & -\frac{1}{\rho_0} & \frac{1}{\rho_0} & 0 \\ 0 & \frac{T_0}{c_v^*} & 0 & 0 & 0 & \frac{1}{4ac_v^*\rho_0} \\ 0 & -\frac{4}{3}a\rho_0T_0 & 0 & 0 & 0 & -\frac{3(1+c_v^*)}{2c_v^*-3} \\ 0 & \left(\frac{2}{3} - \frac{1}{c_v^*}\right)a\rho_0T_0 & 0 & 0 & 0 & \frac{3c_v^*(1+c_v^*)}{3c_v^*(1+c_v^*)} \\ 0 & 0 & (1+c_v^*)a^2\rho_0T_0 & -aT_0 & aT_0 & 0 \end{pmatrix} \quad \text{and} \quad (8)$$

$$\mathbf{B}_0 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{\tau_S} & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{\tau_{\Pi}} \\ 0 & 0 & 0 & 0 & -\frac{1}{\tau_q} \end{pmatrix}. \quad (9)$$

3 Dispersion relation for sound

In this section, we deduce the dispersion relation, and then obtain the high-frequency limit of the phase velocity and the attenuation factor.

3.1 Dispersion relation, phase velocity and attenuation factor

We study a plane harmonic wave propagating in the positive x -direction with the frequency ω and the complex wave number $k = k_r + ik_i$ ($k_r = \Re(k)$, $k_i = \Im(k)$) such that

$$\mathbf{u} = \mathbf{w}e^{i(\omega t - kx)}, \quad (10)$$

where \mathbf{w} is a constant amplitude vector. From Eq. (7), the dispersion relation is expressed by [13]:

$$\det \left(\mathbf{I} - z\mathbf{A}_0 + \frac{i}{\omega}\mathbf{B}_0 \right) = 0, \quad (11)$$

where $z \equiv k/\omega$ and \mathbf{I} is the unit matrix. Then the phase velocity v_{ph} and the attenuation factor α are calculated as the functions of the frequency ω :

$$v_{ph}(\omega) = \frac{\omega}{\Re(k)} = \frac{1}{\Re(z)}, \quad (12)$$

$$\alpha(\omega) = -\Im(k) = -\omega\Im(z). \quad (13)$$

By introducing the dimensionless parameters defined by

$$\Omega = \tau_S \omega, \quad \tau_{qs} = \frac{\tau_q}{\tau_S}, \quad \tau_{ps} = \frac{\tau_{ps}}{\tau_S}, \quad (14)$$

the dispersion relation (11) is shown explicitly as

$$\begin{aligned} & \frac{c_v^* (c_0 z)^4}{3\Omega^2 (1 + c_v^*)^2 \tau_{ps}} \left(-3(1 + c_v^*) - i\Omega (3 + 7c_v^* + 5c_v^* \tau_{ps}) + 9\Omega^2 c_v^* \tau_{ps} \right) \\ & + \frac{(c_0 z)^2}{3\Omega^3 (1 + c_v^*)^2 \tau_{qs} \tau_{ps}} \left[-3i(1 + c_v^*)^2 + \Omega(1 + c_v^*) (3 + 7c_v^* + 5c_v^* \tau_{ps} + 6(1 + c_v^*) \tau_{qs}) \right. \\ & \left. + i\Omega^2 \left(2(3 + 10c_v^* + 5c_v^{*2}) \tau_{qs} + 9c_v^* (1 + c_v^*) \tau_{ps} + c_v^* (13 + 8c_v^*) \tau_{qs} \tau_{ps} \right) - 3\Omega^3 c_v^* (7 + 4c_v^*) \tau_{ps} \tau_{qs} \right] \\ & + \frac{(\Omega - i)(\tau_{ps} \Omega - i)(\tau_{qs} \Omega - i)}{\Omega^3 \tau_{ps} \tau_{qs}} = 0 \end{aligned} \quad (15)$$

with c_0 being the sound velocity in equilibrium:

$$c_0 = \sqrt{\left(\frac{\partial p}{\partial \rho} \right)_0 + \frac{T_0 \left(\frac{\partial p}{\partial T} \right)_0^2}{\rho_0^2 \left(\frac{\partial \varepsilon}{\partial T} \right)_0}} = \sqrt{aT_0 \left(1 + \frac{1}{c_v^*} \right)}, \quad (16)$$

where the suffix 0 indicates the values at the reference equilibrium state. Therefore, for given c_v^* , τ_{qs} and τ_{ps} , the quantity $c_0 z (= c_0 k / \omega)$ is calculated from Eq. (15) as the function of $\Omega (= \tau_S \omega)$. Hereafter in the present paper, we will confine our study within the *fastest* sound wave because the experiments discussed in Sect. 4 give us the data on this wave.

3.2 High frequency limit of the phase velocity and the attenuation factor

From the general theory [1, 13], we have the relations:

$$v_{ph}^{(\infty)} \equiv \lim_{\omega \rightarrow \infty} v_{ph}(\omega) = \lambda_0, \quad (17)$$

$$\alpha^{(\infty)} \lambda_0 \equiv \lim_{\omega \rightarrow \infty} \alpha(\omega) \lambda_0 = -\mathbf{l}_0 \cdot \mathbf{B}_0 \cdot \mathbf{d}_0, \quad (18)$$

where the characteristic velocity λ_0 is the largest eigenvalue of \mathbf{A}_0 , and \mathbf{l}_0 and \mathbf{d}_0 are the corresponding left and right eigenvectors of \mathbf{A}_0 . Then we obtain the limits in the present case:

$$v_{ph}^{(\infty)} = \sqrt{\frac{aT_0(4c_v^* + 7 + F)}{2(1 + c_v^*)}}, \quad (19)$$

$$\alpha^{(\infty)} = \frac{\sqrt{2(1 + c_v^*)^3 (F(4 + c_v^*) - 22 - 11c_v^* + 2c_v^{*2})}}{9c_v^* \tau_S \sqrt{aT_0} \sqrt{7 + 4c_v^* + F} (7 + 4c_v^* - F)^2 F} \left(4c_v^* + \frac{3c_v^* (8 + 2c_v^* - F)}{\tau_{qs}} + \frac{-3 + 2c_v^*}{\tau_{ps}} \right), \quad (20)$$

where F is given by

$$F = \sqrt{37 + 32c_v^* + 4c_v^{*2}}. \quad (21)$$

The dependence of the phase velocity $v_{ph}^{(\infty)}$ on c_v^* is shown in Fig. 1. In a rarefied monatomic gas with $c_v^* = 3/2$, the phase velocity $v_{ph}^{(\infty)}$ is given by $2.13051\sqrt{aT_0}$ [1]. For large c_v^* , it approaches $\sqrt{3aT_0}$. On the other hand, the attenuation factor $\alpha^{(\infty)}$

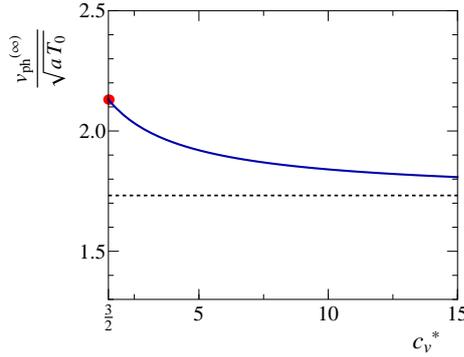


Fig. 1 Dependence of the phase velocity in the high frequency limit $v_{ph}^{(\infty)}$ on the dimensionless specific heat c_v^* . Rarefied monatomic gases correspond to the case with $c_v^* = 3/2$. The dotted line is the asymptote.

depends not only on c_v^* but also on the relaxation times. In a rarefied monatomic gas, the attenuation factor $\alpha^{(\infty)}$ is given by $(0.0951852 + 0.0931368/\tau_{qs}) / (\tau_S \sqrt{aT_0})$ [1]. For large c_v^* , it approaches $(1 + 2\tau_{ps}) / (9\sqrt{3}\tau_{ps}\tau_S \sqrt{aT_0})$.

4 Comparison with experimental data

The dispersion relation obtained above, in particular, the phase velocity v_{ph} and the attenuation factor α as the functions of the frequency ω are compared with the experimental data on normal hydrogen (n-H₂), para hydrogen (p-H₂), normal deuterium (n-D₂), ortho deuterium (o-D₂) and hydrogen deuteride (HD) gases at temperatures 77.3K, 90.2K and the room temperatures [14,15]. The comparison is also made with the predictions by the classical NSF theory.

Before discussing the subject, we need to make preliminary calculations for determining the values of c_v^* , τ_{qs} and τ_{ps} defined in (4) and (14) at the reference equilibrium state.

4.1 Preliminary calculations

4.1.1 Specific heat

We calculate the specific heat c_v^* of hydrogen, deuterium and hydrogen deuteride gases on the basis of statistical mechanics [16,17]. As we may safely neglect the contribution of internal vibrational modes in a molecule to the specific heat in the temperature range under consideration, we take only the translational and rotational modes into account. We assume also that the translational mode satisfies the equipartition law of energy. Then c_v^* is expressed as

$$c_v^* = \frac{3}{2} + c_{v,\text{rot}}^*, \quad c_{v,\text{rot}}^* = \beta^2 \frac{\partial^2 \log Z_{\text{rot}}}{\partial \beta^2}, \quad (\beta \equiv \frac{1}{k_B T}) \quad (22)$$

where $c_{v,\text{rot}}^*$ and Z_{rot} are the specific heat and the partition function due to the rotational modes.

For gases composed of heteronuclear diatomic molecules (HD), the partition function is given by

$$Z_{\text{rot}} = \sum_{l=0}^{\infty} (2l+1) \exp[-\beta B l(l+1)], \quad (23)$$

where l is the quantum number of the orbital angular momentum and $B = \hbar^2/2I$ with I and \hbar being the moment of inertia of a molecule and the Planck constant divided by 2π , respectively. While, for gases composed of diatomic homonuclear molecules (H_2 and D_2), the partition function is given by

$$\begin{aligned} Z_{\text{rot}} &= Z_g^{g_g} Z_u^{g_u}, \\ Z_g &= \sum_{l=\text{even}} (2l+1) \exp[-\beta B l(l+1)], \\ Z_u &= \sum_{l=\text{odd}} (2l+1) \exp[-\beta B l(l+1)], \end{aligned} \quad (24)$$

where g_g and g_u are defined by

$$\text{H}_2 \begin{cases} \text{normal} - \text{H}_2 : g_u = 3/4, g_g = 1/4 \\ \text{para} - \text{H}_2 : g_u = 0, g_g = 1 \end{cases}, \quad \text{D}_2 \begin{cases} \text{normal} - \text{D}_2 : g_u = 1/3, g_g = 2/3 \\ \text{ortho} - \text{D}_2 : g_u = 0, g_g = 1 \end{cases}. \quad (25)$$

Numerically calculated values of c_v^* are shown in Table 1 and in Fig. 2. The values of B of H_2 , D_2 and HD adopted are 12.09×10^{-22} [J], 6.047×10^{-22} [J] and 9.068×10^{-22} [J], respectively [18].

4.1.2 Relaxation times

From (5), we have the following relations for the ratios τ_{qs} and τ_{ps} :

$$\tau_{qs} = (1 + c_v^*)^{-1} \frac{\kappa}{a\mu}, \quad (26)$$

$$\tau_{ps} = \left(\frac{2}{3} - \frac{1}{c_v^*} \right)^{-1} \frac{\nu}{\mu}. \quad (27)$$

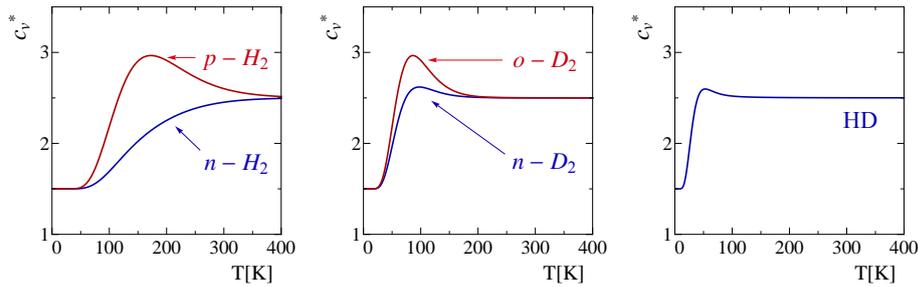


Fig. 2 Dependence of the dimensionless specific heat c_v^* for n-H₂ and p-H₂ (left), n-D₂ and o-D₂ (center), and HD (right) on the temperature T .

Therefore, in principle, with the help of the experimental data on μ , κ and ν , we can estimate the values of τ_{qs} and τ_{ps} . However, at present, as we have the reliable data only on μ and κ [15], we adopt, in the analysis below, an adjustable parameter:

$$\varphi = \frac{\nu}{\mu}. \quad (28)$$

We summarize the adopted values of c_v^* , c_0 , μ , κ , τ_{qs} and the evaluated values of φ and τ_{ps} in Table 1, details of which will be discussed in the next subsection.

4.2 Experimental data and theoretical predictions for the dispersion relation

4.2.1 Hydrogen gases: n-H₂ and p-H₂

For n-H₂, the dimensionless phase velocity, v_{ph}/c_0 , and the dimensionless attenuation factor, $c_0\tau_S\alpha$, are shown as the functions of the dimensionless frequency Ω in Fig. 3. We see the experimental data on the phase velocity at $T_0 = 273.5, 296.8\text{K}$ by Rhodes [14] and on the attenuation factor at $T_0 = 293\text{K}$ by Sluijter et al. [15] accompanied by the theoretical results at $T_0 = 293\text{K}$ predicted by the ET theory and the NSF theory.

Noticeable points from Fig. 3 are summarized as follows: (i) In the region with small Ω , as is expected, the predictions by the two theories coincide with each other. The value of the parameter φ is determined to be 37 as the best fit with the experimental data in this region. This procedure of determining φ will be adopted throughout the present paper. (ii) When we go into the ultrasonic frequency region with larger Ω , the prediction by the ET theory is evidently superior to that by the NSF theory. The difference between the two theories emerges around $\Omega = \omega\tau_s = 10^{-3}$. We will evaluate τ_s , which depends on T_0 and p_0 , later. (iii) The ET theory seems to be valid at least up to the experimental data with the maximum dimensionless frequency $\Omega = 10^{-1}$. (iv) The large value of φ means that $\nu \gg \mu$. We will discuss its physical meaning below.

For p-H₂, we compare the theoretical predictions with the experimental data on the phase velocity at $T_0 = 273.8, 298.4\text{K}$ by Rhodes [14] and on the attenuation

Table 1 Values of the temperature T_0 , dimensionless specific heat c_v^* , sound speed in equilibrium c_0 , shear viscosity μ [15], heat conductivity κ [15] and the ratio of the relaxation times of the heat flux and the deviatoric part of the viscous stress τ_{qs} adopted in the present analysis. And the values of the parameter φ , bulk viscosity ν , and the ratio of the relaxation times of the bulk viscosity and the deviatoric part of the viscous stress τ_{ps} evaluated by the present analysis.

Gas	T_0 [K]	c_v^*	c_0 [$\frac{m}{s}$]	μ [$\mu\text{Pa}\cdot\text{s}$]	κ [$\frac{mW}{m\cdot K}$]	τ_{qs}	φ	ν [$\mu\text{Pa}\cdot\text{s}$]	τ_{ps}
n - H ₂	77.3	1.57	723	3.50	49.8	1.34	28	98.0	988
	293	2.45	1300	8.82	182	1.46	37	326	144
p - H ₂	77.3	1.76	707	3.50	52.7	1.33	76	266	783
	90.2	1.99	748	3.97	63.6	1.30	76	302	465
	293	2.61	1290	8.82	192	1.46	31	273	109
n - D ₂	77.3	2.54	472	4.82	45.6	1.30	36	174	132
	293	2.50	920	12.3	131	1.47	22	271	82.5
o - D ₂	77.3	2.93	463	4.82	49.4	1.26	44	212	135
	90.2	2.96	499	5.50	55.6	1.24	33	182	100
	293	2.50	920	12.3	131	1.47	22	271	82.5
HD	77.3	2.55	544	4.21	51.9	1.26	1.4	5.89	5.11
	293	2.50	1060	10.8	149	1.43	2.4	25.9	8.99

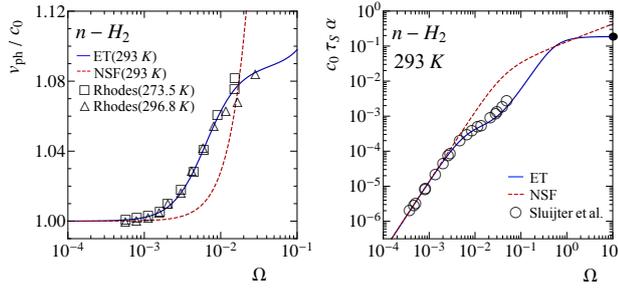


Fig. 3 Dependence of the dimensionless phase velocity v_{ph}/c_0 (left) and the attenuation factor $c_0\tau_S\alpha$ (right) on the dimensionless frequency Ω for n-H₂. The squares and triangles in the left figure are the experimental data at $T_0 = 273.5$ and 296.8 K, respectively, by Rhodes [14], and the circles in the right figure are those at $T_0 = 293$ K by Sluijter et al. [15]. The solid and dashed lines are predictions at 293K by the ET and NSF theories, respectively. The black circle on the right vertical line in the right figure corresponds to $\alpha^{(\infty)}$. We adopt $\varphi = 37$.

factor at $T_0 = 293$ K by Sluijter et al. [15]. We have a similar result as shown in Fig. 4, where the selected value of the parameter φ is 31. Remarkable points in this case are qualitatively the same as in the case of n-H₂ above.

Hereafter we focus our discussion only on the attenuation factor because of the lack of the experimental data on the phase velocity for the purpose of the present study. In Fig. 5, the attenuation factors for n-H₂ at $T_0 = 77.3$ K and for p-H₂ at

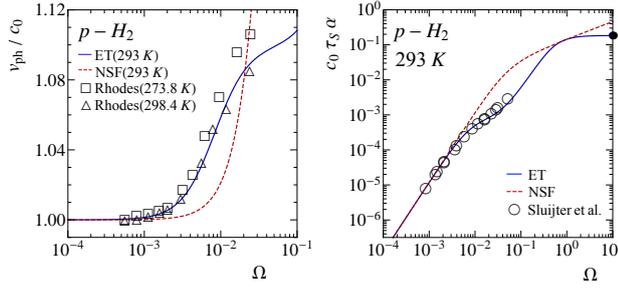


Fig. 4 Dependence of the dimensionless phase velocity v_{ph}/c_0 (left) and the attenuation factor $c_0 \tau_S \alpha$ (right) on the dimensionless frequency Ω for p- H_2 . The squares and triangles in the left figure are the experimental data at $T_0 = 273.8$ and 298.4 K, respectively, by Rhodes [14], and the circles in the right figure are those at $T_0 = 293$ K by Sluijter et al. [15]. The solid and dashed lines are predictions at 293K by the ET and NSF theories, respectively. The black circle on the right vertical line in the right figure corresponds to $\alpha^{(\infty)}$. We adopt $\varphi = 31$.

$T_0 = 77.3, 90.2$ K are shown. We see again that the present theory can describe the experimental data very well. The values of the parameter φ are selected to be 28, 76 and 76, respectively. These values are again very large.

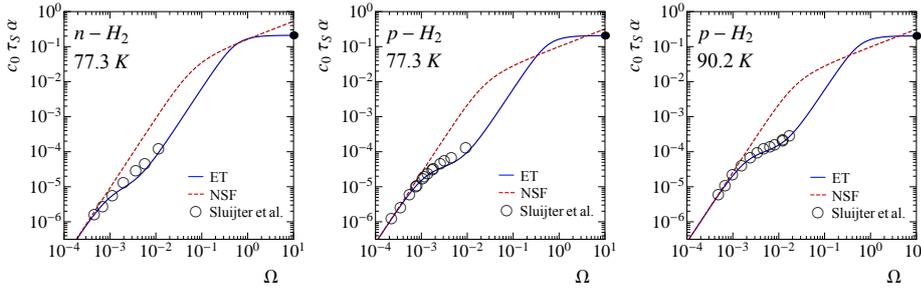


Fig. 5 Dependence of the dimensionless attenuation factor $c_0 \tau_S \alpha$ on the dimensionless frequency Ω for n- H_2 at $T_0 = 77.3$ K (left), and for p- H_2 at $T_0 = 77.3$ K (center) and 90.2 K (right). The circles are the experimental data by Sluijter et al. [15]. The solid and dashed lines are predictions by the ET and NSF theories, respectively. The black circle on the right vertical line in each figure corresponds to $\alpha^{(\infty)}$. We adopt $\varphi=28, 76$ and 76 from left to right.

4.2.2 Deuterium gases: n- D_2 and o- D_2

Comparisons are also made for n- D_2 at $T_0 = 77.3$ and 293 K with $\varphi=36$ and 22 in Fig. 6, and for o- D_2 at $T_0 = 77.3, 90.2$ and 293 K with $\varphi=44, 33$ and 22 in Fig. 7. From these figures, we have qualitatively the same observations as those in the case of hydrogen gases.

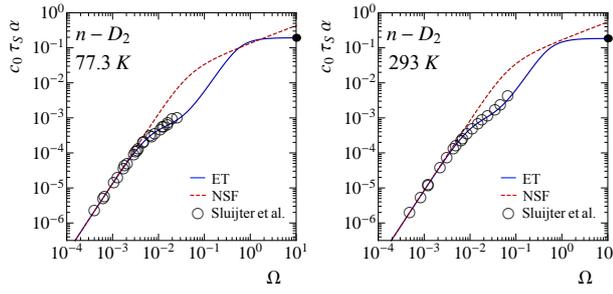


Fig. 6 Dependence of the dimensionless attenuation factor $c_0\tau_S\alpha$ on the dimensionless frequency Ω for n- D_2 at $T_0=77.3\text{K}$ (left) and 293K (right). The circles are the experimental data by Sluijter et al. [15]. The solid and dashed lines are predictions by the ET and NSF theories, respectively. The black circle on the right vertical line in each figure corresponds to $\alpha^{(\infty)}$. We adopt $\varphi=36$ (left) and 22 (right).

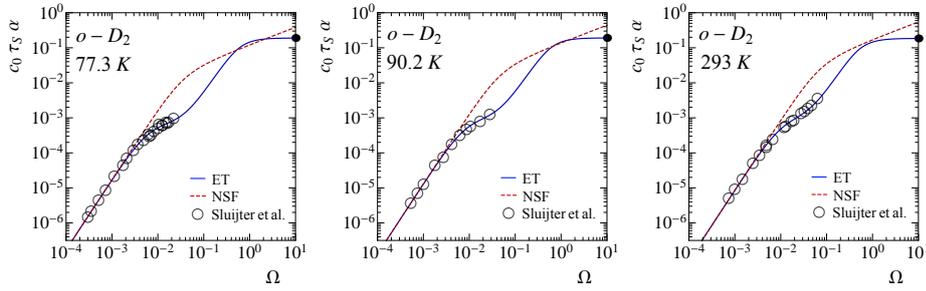


Fig. 7 Dependence of the dimensionless attenuation factor $c_0\tau_S\alpha$ on the dimensionless frequency Ω for o- D_2 at $T_0 = 77.3\text{K}$ (left), 90.2K (center) and 293K (right). The circles are the experimental data by Sluijter et al. [15]. The solid and dashed lines are predictions by the ET and NSF theories, respectively. The black circle on the right vertical line in each figure corresponds to $\alpha^{(\infty)}$. We adopt $\varphi = 44, 33$ and 22 from left to right.

4.2.3 Hydrogen deuteride gases: HD

Lastly we show the results of HD gases at $T_0 = 77.3$ and 293K in Fig. 8. We notice the following points: (i) The difference between the two theories is small and the theoretical predictions are consistent with the experimental data in the range: $\Omega \leq 10^{-1}$. This means that the local equilibrium assumption holds well up to $\Omega \cong 10^{-1}$, while for the other gases analyzed above the assumption holds until $\Omega \cong 10^{-3}$. (ii) The values of φ adopted here are 1.4 and 2.4 . These values are $O(1)$, that is, $\nu \sim \mu$, and are very small compared with those obtained for the other gases discussed above. We will discuss this interesting fact below.

4.3 Remarks

Three remarks (A)-(C) are made below.

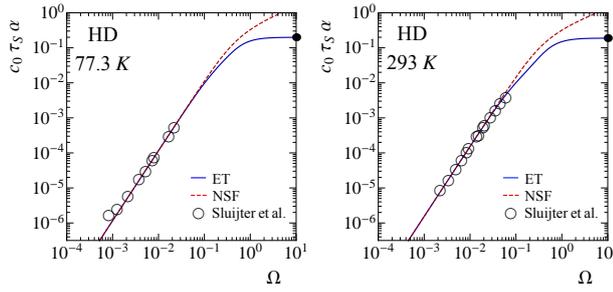


Fig. 8 Dependence of the dimensionless attenuation factor $c_0 \tau_S \alpha$ on the dimensionless frequency Ω for HD at $T_0=77.3\text{K}$ (left) and 293K (right). The circles are the experimental data by Sluijter et al. [15]. The solid and dashed lines are predictions by the ET and NSF theories, respectively. The black circle on the right vertical line in each figure corresponds to $\alpha^{(\infty)}$. We adopt $\varphi = 1.4$ (left) and 2.4 (right).

(A) We have seen clearly that the present theory of ET is consistent with the experimental data even in the high frequency range where the local equilibrium assumption is no more valid. Although the comparisons with the experimental data have been made only for the rarefied diatomic gases, the consistency gives us a strong confidence that the ET theory for dense gases [2] deserves further studies. There are potentially many research fields where the ET theory may play a crucial role, for example, fields of acoustics [19] and gas dynamics [20].

(B) From the values of the ratios τ_{qs} and τ_{ps} in Table 1, we have noticed an interesting fact that, except for HD gases, τ_{II} is much larger than τ_S , while τ_S and τ_q are comparable with each other. This fact was reported also in some kinetic theoretical studies [21, 22]. By using the result summarized in Table 2, the relaxation times for given T_0 and p_0 can be estimated. For example, the relaxation times in a n- H_2 gas at $p_0 = 10^3$ [Pa] and $T_0 = 77.3$ [K] can be calculated: $\tau_S = 3.50 \times 10^{-9}$ [s], $\tau_{II} = 3.46 \times 10^{-6}$ [s] and $\tau_q = 4.70 \times 10^{-9}$ [s].

In a preceding paper [23], it was pointed out that the relaxation time τ_{II} is in the same order of magnitude as the relaxation time of the energy exchange between the molecular translational mode and the internal modes, which, in the present case, are the rotational modes. The results obtained above suggest that the sharp temperature change of the specific heat due to the rotational modes $c_{v,\text{rot}}^*$ depicted in Fig. 2 is somehow related to the emergence of the large value of τ_{II} . The detailed study of this subject is, however, beyond the scope of the present phenomenological study, and its statistical-mechanical or kinetic-theoretical study by taking into account the realistic collision processes between the constituent molecules is required.

(C) From the values of φ in Table 1, we have also noticed a similar fact that, except for HD gases, the bulk viscosity ν is much larger than the shear viscosity μ . The similarity is natural because there are relations between the viscosities and the relaxation times as shown in Eq. (5). A point to be emphasized here is that, as the direct experiments to measure the bulk viscosity are usually difficult, the method for the evaluation of the bulk viscosity utilized here through analyzing the dispersion relation on the basis of the ET theory is quite useful. The values of ν

Table 2 Relaxation times of the deviatoric part of the viscous stress τ_S , dynamic pressure τ_{II} and heat flux τ_q multiplied by the pressure p_0 for several values of T_0 in H_2 , D_2 and HD gases.

Gas	T_0 [K]	$\tau_S p_0$ [s · μ Pa]	$\tau_{II} p_0$ [s · μ Pa]	$\tau_q p_0$ [s · μ Pa]
n – H_2	77.3	3.50	3460	4.70
	293	8.82	1270	12.8
p – H_2	77.3	3.50	2740	4.64
	90.2	3.97	1850	5.16
	293	8.82	962	12.9
n – D_2	77.3	4.82	637	6.25
	293	12.3	1010	18.1
o – D_2	77.3	4.82	652	6.09
	90.2	5.50	552	6.81
	293	12.3	1010	18.1
HD	77.3	4.21	21.5	5.32
	293	10.8	97.1	15.5

thus evaluated are summarized in Table 1. We hope that present thermodynamic approach contributes to the recent studies of the bulk viscosity [24–28].

5 Summary and concluding remarks

To sum up, we have studied the dispersion relations in rarefied polyatomic gases, that is, hydrogen, deuterium and hydrogen deuteride gases, basing on the ET theory of dense gases. We have properly taken the temperature dependence of the specific heats, c_v , of these gases into the dispersion relations. The comparison of the theoretical predictions with experimental data on the phase velocity and the attenuation factor has revealed that the ET theory is valid even in nonequilibrium states out of local equilibrium. We have also evaluated the bulk viscosity and the relaxation times.

Finally some concluding remarks are made:

(i) There is a phenomenological theory of the dispersion relation for sound, the basic equations of which are composed of the relaxation equations for some nonequilibrium parameters and the Euler (or NSF) equations for the conservation laws [10, 29]. One crucial point is that the theory is based on the local equilibrium assumption. In this respect, this may be regarded as a theory in the framework of thermodynamics of irreversible processes [10]. Because of this, in the present paper, we have compared the ET theory only with the NSF theory as a representative one. In Ref. [23], the relationship between the simplified ET theory and the theory with one relaxation equation was studied in detail.

(ii) We have analyzed the experimental data on rarefied hydrogen, deuterium and hydrogen deuteride gases in the temperature range where the rotational modes

in a molecule play an important role. The ET theory can be applied to many other rarefied polyatomic gases in a wider temperature range where the rotational and/or vibrational modes in a molecule play a role. Comprehensive study of this must be a promising future work.

(iii) As is mentioned in the first section, it is interesting to study the dispersion relation for sound in dense gases. As a first step, we are now studying it in a gas prescribed by the virial equations of state. The result will soon be reported.

(iv) In order to study the effect of the large value of the relaxation time τ_{II} on various nonequilibrium phenomena such as shock wave phenomena, it seems to be appropriate to adopt a simpler model than the one adopted here. The theory with only 6 independent field variables (ρ, v_i, T, II) developed in [23] may play an important role in such studies.

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