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Ultrasound propagation studied using the discrete kinetic theory

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Abstract. We use discrete kinetic models to study the dispersion relations of the one-dimensional plane-ultrasound-wave propagation in monatomic gases, which are fundamental in non-equilibrium statistical thermodynamics. The results show that six- and eight-velocity models can capture the propagation of the diffusion mode, which has not been reported on since 1965. A four-velocity model is seen to capture the propagation of the sound mode in the higher-Knudsen-number regime quite well when we compare our calculated results on the dispersion (phase speed and absorption) relations with Greenspan's measurements.

1. Introduction

There have been several investigations (measurements and theoretical papers [1–7]) concerned with the analysis of the propagation of very high-frequency plane sound waves. Most of them were numerical approaches, and are related to the initial-value problem for an unbounded domain. Their aim was to describe the sound propagation for all ratios of the mean free path to the sound wavelength. Ultrasound propagation in highly rarefied monatomic gases, i.e., gases in which the ratio of the collision to the sound frequency $h = p_0/\omega\mu$ is small (h is usually termed the *rarefaction parameter*, and is the inverse of the Knudsen number K_n, defined as the mean free path of the gas divided by the sound wavelength; p_0 is the reference pressure; μ is the viscosity of the gas; ω is the circular oscillation frequency), had been studied by using the linearized Boltzmann equation as the dispersion relation (i.e., describing the velocity of propagation and the absorption of sound) in the early 1960s [8–10]. Considering the linearized Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \boldsymbol{x}} = \mathcal{L}[f]$$

(where $f \equiv f(\boldsymbol{\xi}, \boldsymbol{x}, t)$ is the continuous molecular distribution function, $\boldsymbol{\xi}$ denotes the continuous molecular velocity, $\mathcal{L}$ is the linearized collision operator), regarding the nature of intermolecular and/or molecule–surface collisions, it is convenient to consider the problem in three distinct regimes of pressure which could also be classified according to the Knudsen number (K_n) [6]:

(1) *The classical regime*. Quantities vary little over the mean free path or the mean time of intermolecular collisions. Moreover, molecule–surface effects are quite negligible even at short distances from the transmitter.

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(2) *The frequency relaxation regime*. The frequency of intermolecular collisions f_c is comparable to or smaller than the frequency $\omega/2\pi$ of the sound field. This regime is not well defined unless the sound field is observed at large distances from the transmitter surface.
(3) *The geometrical relaxation regime*. The molecules are assumed to traverse the path from the transmitter to the receiver control surface essentially without undergoing any intermolecular collisions.

The solution of the continuous Boltzmann equation depends primarily on the molecule–surface interaction even though this term can only be approximately formulated. The kinetic theory of gases has developed differently for neutral systems and fully ionized plasmas. The major reason for this is that collisions are typically far more important in neutral gases or weakly ionized plasmas than fully ionized plasmas. Consequently, the handling of the Boltzmann collision integral is central to these theories. For the problem of the propagation of sound in monatomic gases, we normally seek solutions for f of the form

$$f = f_0\{1 + \phi(\boldsymbol{\xi}) \exp[\mathrm{i}(\boldsymbol{k} \cdot \boldsymbol{x} - \omega t)]\}$$

where f_0 is the Maxwellian distribution, ϕ is a small perturbation ($\phi \ll 1$), and $\boldsymbol{k}$ is the wavenumber.

It is difficult to assess their accuracy of those previous numerical attempts since they are essentially *ad hoc* and insensitive to the many singular features of the solution. For example, a polynomial approximation in the neighbourhood of a free flow was described by Kahn and Mintzer [7]; this is much more likely to give an accurate representation in the high-frequency regime, but again the error is hard to estimate and not all singular features are visible. Pekeris *et al* [8] used the higher-order moment and polynomial approximations only for the linearized Boltzmann collision operator and neglected the contributions of the higher molecular velocities. Sirovich and Thurber [9] only evaluated the normal modes and did not solve the boundary value problem [10].

With extended irreversible/reversible thermodynamics (EIT), however, researchers could also study the ultrasound propagation in rarefied gases by including the time relaxation effects in the classical Navier–Stokes–Fourier approaches [11] for the heat flux and viscous pressure (which are of the order of the collision time). They just carefully made *ad hoc* adjustments to the constants of the time relaxation for different physical applications. The approach is not universal but depends on the specific problem considered.

Recently microtechnology and nanotechnology have produced many built-in sensors in sub-micron (microchannels) or atomic-scale (nanochannels) environments by the use of surface micromachining or other advanced processings. For example, researchers can put many pressure sensors, streamwise and staggered, along the walls of the microchannel in order to measure the pressure distribution along the channel [12]. In this situation, if the flowing fluids are monatomic gases, the propagation of sound waves in this microchannel will be an interesting problem which is similar to that of ultrasound propagation in rarefied gases [13]. Considering the complicated geometry near the walls, however—as there are many built-in sensors along the walls—the boundary conditions are too difficult to apply for solving the problem [14, 15]. We thus only consider the 1D propagation of plane sound waves near the centreline region of the microchannel, neglecting the complicated real boundary conditions at the walls and the transmitter/receivers.

The velocity of propagation of a sound wave can be classically determined by looking for the properties of the solutions of the conservation equations referred to the Maxwellian state. Recently some researchers used discrete [16, 17] or semidiscrete [18, 19] Boltzmann models to study the 1D ultrasound propagation by calculating the speed of sound [16, 18] or the dispersion relations [19]. Discrete velocity models were applied in the late 1970s for

solving the discrete Boltzmann equation (DBE) which describes the time evolution of the distribution function, giving the probability density of finding the dilute gas molecule in space and time [20]. The primary approach is to use the discrete velocity instead of the continuous velocity of the corresponding molecular distribution. To replace the continuous Boltzmann equation (CBE), which is required whenever the mean free path of the gas molecules is not negligible in comparison with the length scale of the problem considered, mathematical and physical aspects of the DBE were intensively investigated again in the late 1980s [21].

In this presentation, we shall use the generalized $2n$-velocity ($n = 2, 3, 4$) models developed by Gatignol [20] to investigate the kinetic effects of the ultrasound propagation in rarefied gases.

2. Formulations

The discrete Boltzmann equation is a mathematical model in the discrete kinetic theory of gases, which defines the time–space evolution of a system of gas particles with a finite number of velocities $\boldsymbol{v}_i$, $i = 1, \ldots, p$. This model has the structure of a system of semilinear partial differential equations of hyperbolic type that defines the evolution of the discrete number densities $\boldsymbol{N}_i = N_i(t, \boldsymbol{x})$. The simplified model, by considering only binary collisions—i.e. the $(2 \times n)$-velocity model—is concerned with a one-component discrete velocity gas such that the molecules can attain $2n$ velocities in the xy-plane. In particular, the velocity discretization is characterized by

(i) $|\boldsymbol{v}_i| = c$,
(ii) $\boldsymbol{v}_i + \boldsymbol{v}_{i+n} = 0$,
(iii) $\boldsymbol{v}_i \cdot \boldsymbol{v}_{i+1} = c^2 \cos(\pi/n)$ where $i = 1, \ldots, 2n$,

where the index is modulo $2n$, i.e. $i \equiv i + 2n$. Such a model is called a planar $2n$-velocity model. If only binary, elastic collisions are taken into account, then the non-trivial admissible ones (where this term is used to denote those collisions which produce non-vanishing terms in the collision operator) are

head-on collisions $\qquad (\boldsymbol{v}_i, \boldsymbol{v}_{i+n}) \longleftrightarrow (\boldsymbol{v}_j, \boldsymbol{v}_{j+n}) \qquad \forall j \neq i, i = 1, \ldots, 2n.$

Also, the momentum and energy are conserved:

$$\boldsymbol{v}_i + \boldsymbol{v}_{i+n} = \boldsymbol{v}_j + \boldsymbol{v}_{j+n}$$
$$|\boldsymbol{v}_i|^2 + |\boldsymbol{v}_{i+n}|^2 = |\boldsymbol{v}_j|^2 + |\boldsymbol{v}_{j+n}|^2.$$

Moreover, all of the velocity directions after collisions are assumed to be equally probable.

For example, the four-velocity coplanar model that we shall use here is $\boldsymbol{v}_i$, $i = 1, 2, 3, 4$, with

$$\boldsymbol{v}_1 + \boldsymbol{v}_3 = \boldsymbol{v}_2 + \boldsymbol{v}_4$$
$$(\boldsymbol{v}_1 - \boldsymbol{v}_3)^2 = (\boldsymbol{v}_2 - \boldsymbol{v}_4)^2 = 4c^2$$
$$(\boldsymbol{v}_1 - \boldsymbol{v}_3) \cdot (\boldsymbol{v}_2 - \boldsymbol{v}_4) = 0.$$

In this way, considering binary collisions only, the model of the discrete Boltzmann equation proposed in [20] is a system of $2n$ semilinear partial differential equations of the hyperbolic type:

$$\frac{\partial}{\partial t} N_i + \boldsymbol{v}_i \cdot \frac{\partial}{\partial \boldsymbol{x}} N_i = \frac{2cS}{n} \sum_{j=1}^{n} N_j N_{j+n} - N_i N_{i+n} \qquad i = 1, \ldots, 2n \qquad (1)$$

where $N_i = N_{i+2n}$ are unknown functions, and $\boldsymbol{v}_i = c(\cos[(i-1)\pi/n], \sin[(i-1)\pi/n])$; c is the reference velocity modulus; S is an effective collision cross-section [20].

We linearize the above equations around a uniform Maxwellian state (N_0) by setting

$$N_i(t, \boldsymbol{x}) = N_0(1 + P_i(t, \boldsymbol{x}))$$

where P_i is a small perturbation. The linearized version of the above equations is

$$\frac{\partial}{\partial t} P_m + \boldsymbol{v}_m \cdot \frac{\partial}{\partial \boldsymbol{x}} P_m + 2cSN_0(P_m + P_{m+n}) = \frac{2cSN_0}{n} \sum_{k=1}^{2n} P_k. \tag{2}$$

Here, $m = 1, \ldots, 2n$. In these equations, after replacing the index m with $m+n$ and using the identities $P_{m+2n} = P_m$, we have

$$\frac{\partial}{\partial t} P_{m+n} - \boldsymbol{v}_m \cdot \frac{\partial}{\partial \boldsymbol{x}} P_{m+n} + 2cSN_0(P_m + P_{m+n}) = \frac{2cSN_0}{n} \sum_{k=1}^{2n} P_k. \tag{3}$$

Combining the above two equations, firstly adding then subtracting, with $A_m = (P_m + P_{m+n})/2$ and $B_m = (P_m - P_{m+n})/2$, we have

$$\frac{\partial}{\partial t} A_m - c \cos\frac{(m-1)\pi}{n} \frac{\partial}{\partial x} B_m + 4cSN_0 A_m = \frac{4cSN_0}{n} \sum_{k=1}^{2n} A_k \qquad m = 1, \ldots, 2n \tag{4}$$

$$\frac{\partial}{\partial t} B_m + c \cos\frac{(m-1)\pi}{n} \frac{\partial}{\partial x} A_m = 0 \qquad m = 1, \ldots, 2n. \tag{5}$$

From $P_{m+2n} = P_m$, and with $A_m = (P_m + P_{m+n})/2$ and $B_m = (P_m - P_{m+n})/2$, we have $A_{m+n} = A_m$, $B_{m+n} = -B_m$.

After some manipulations, we then have

$$\left[\frac{\partial^2}{\partial t^2} + c^2 \cos^2\frac{(m-1)\pi}{n} \frac{\partial^2}{\partial x^2} + 4cSN_0 \frac{\partial}{\partial t}\right] D_m = \frac{4cSN_0}{n} \sum_{k=1}^{n} \frac{\partial}{\partial t} D_k \tag{6}$$

where $D_m = (P_m + P_{m+n})/2$, $m = 1, \ldots, n$, since $D_1 = D_m$ for $1 = m \pmod{2n}$.

We are ready to look for the solutions in the form of plane waves:

$$D_m = a_m \exp \mathrm{i}(kx - \omega t) \qquad m = 1, \ldots, n$$

with $\omega = \omega(k)$. This is related to the dispersion relations of 1D forced ultrasound propagation of rarefied gases. So we have

$$\left(1 + \mathrm{i}h - 2\lambda^2 \cos^2\frac{(m-1)\pi}{n}\right) a_m - \frac{\mathrm{i}h}{n} \sum_{k=1}^{n} a_k = 0 \qquad m = 1, \ldots, n \tag{7}$$

and

$$\lambda = kc/(\sqrt{2}\omega) \tag{8}$$

where $h = 4cSN_0/\omega \propto 1/K_n$ is the *rarefaction parameter* of the gas; K_n is the Knudsen number which is defined as the ratio of the mean free path of the gases to the wavelength of the ultrasound.

Let

$$a_m = \mathcal{C} \Big/ \left(1 + \mathrm{i}h - 2\lambda^2 \cos^2\frac{(m-1)\pi}{n}\right)$$

where $\mathcal{C}$ is an arbitrary unknown constant, because here we are only interested in the eigenvalues of the above relation. The eigenvalue problems for different $2n$-velocity models reduce to $F_n(\lambda) = 0$, or

$$1 - \frac{\mathrm{i}h}{n} \sum_{m=1}^{n} \frac{1}{1 + \mathrm{i}h - 2\lambda^2 \cos^2((m-1)\pi/n)} = 0. \tag{9}$$

We solve the $n = 2$, 3, and 4 cases separately, i.e., the four-velocity, six-velocity, and eight-velocity cases. The corresponding eigenvalue equations take algebraic polynomial forms [22] with the complex roots being the λ-values.

For the (2×2)-velocity model, we obtain

$$1 - (\mathrm{i}h/2) \sum_{m=1}^{2} [1/\{1 + \mathrm{i}h - 2\lambda^2 \cos^2((m-1)\pi/2)\}] = 0. \tag{10}$$

Likewise, we have, for the (2×3)-velocity model,

$$6\lambda^4 - (15 + 22\mathrm{i}h)\lambda^2 - 8h^2 + 14\mathrm{i}h + 6 = 0 \tag{11}$$

and, for the (2×4)-velocity model,

$$k_0\lambda^8 + k_1\lambda^6 + k_2\lambda^4 + k_3\lambda^2 + k_4 = 0 \tag{12}$$

with

$$k_0 = 4b \qquad k_1 = -12b - 10\hat{c} \qquad k_2 = 13b + 12\hat{c} + 9b\hat{c}$$
$$k_3 = -6b - 10b\hat{c} - 4h^2\hat{c} \qquad k_4 = 3b\hat{c} + \hat{c}^2 b + 3bh^2\hat{c}$$

where $b = 1 + h^2$ and $\hat{c} = 1 - \mathrm{i}h$.

3. Results and discussion

After we obtain the complex roots (λ) for the polynomial equations given above [22], we obtain the values for the (non-dimensional) sound dispersion (real part: λ_i; which is a kind of the measure of the ratio between the propagating and the reference sound speeds) and the attenuation or absorption (imaginary part: λ_i). The spectra of the $(2 \times n)$-velocity models for $n = 2, 3, 4$ look entirely different [21]. To compare with previous results, we have already found the rules of transformation between different researchers' parameters, like h and the inverse Knudsen number. The results for different models are shown in figure 1, with the Navier–Stokes data [2] included for comparison.

We can observe that for the attenuation part, only the results of the four-velocity model show a similar trend (i.e., $O(h^{-2})$) to the Navier–Stokes data as $h \to \infty$. Meanwhile, for the sound dispersion case, once $h \to \infty$, the results for the four-velocity model approach the continuum limit of the sound speed, which is nearly the same as the molecular speed.

To compare with previous experiments by Greenspan [2], we only plot the data from the four-velocity model in figure 2, together with the data obtained from Pekeris *et al* [8] and Lebon and Cloot [23]. Some of the data are also tabulated in table 1 to allow a detailed look. We can observe that the four-velocity model captures the propagating behaviour of the sound mode quite well except for in the $h < 2$ region, while six- and eight-velocity models seem to only capture the propagating mode of diffusion [5, 14, 24–26]. Possible explanations are listed below.

(i) A $2n$-velocity model has only one velocity modulus, which suffers the same limitations as, e.g., the approach of Pekeris *et al*, as was commented on in the introduction. Besides, because of the discrete nature of the four-velocity model, considering the discrete number density, our results underestimated the sound attenuation compared with those from measurements and continuous Boltzmann approaches.

(ii) As the perturbations are relative to the Maxwellians, which are closely related to the macroscopic state variables [21], these results perhaps verify Gatignol's comments on the general $2n$-velocity model that for $n \geqslant 3$, there are more collision invariants than physical

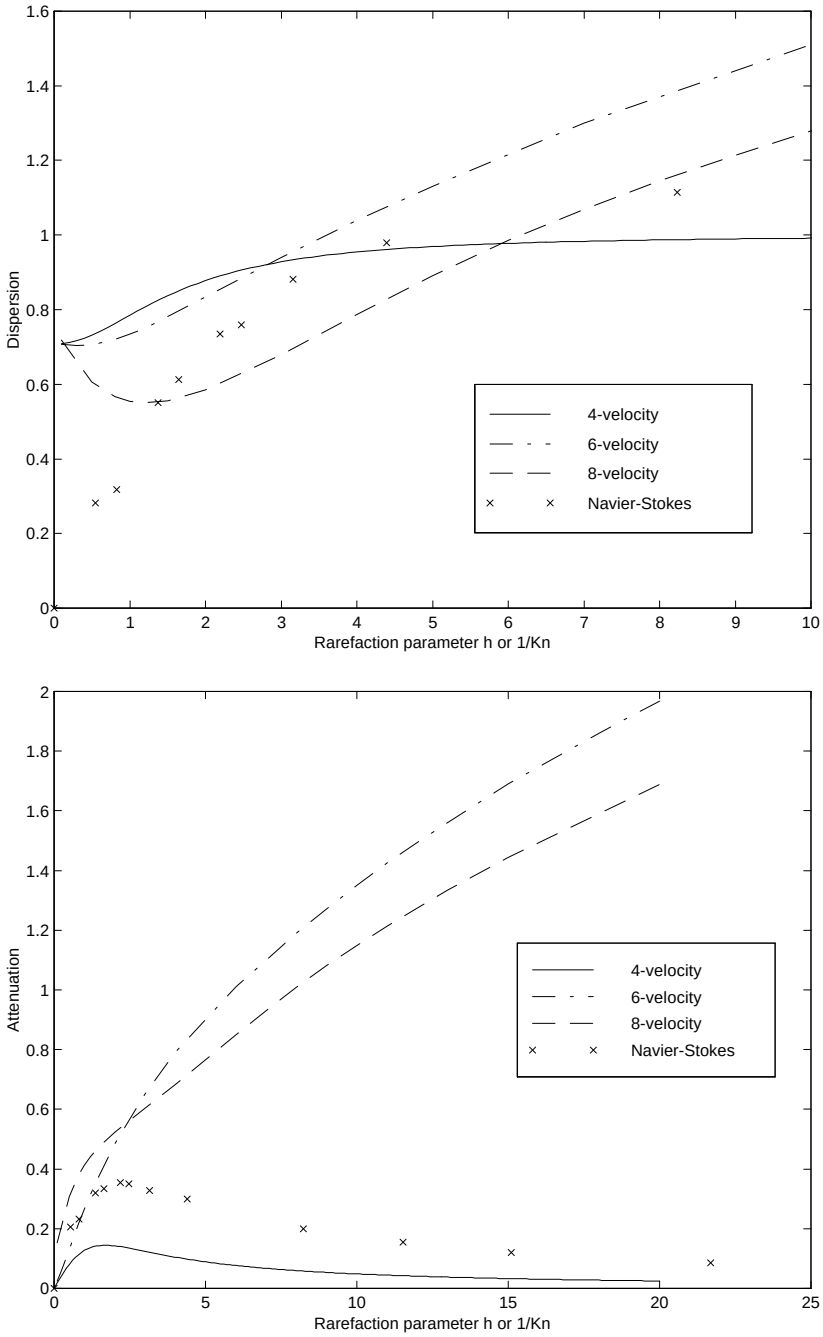

Figure 1. Comparison with the Navier–Stokes approach for the dispersion (upper panel) and attenuation (lower panel) with respect to the rarefaction parameter h. Calculated λ_r: values for the *dispersion*; and λ_i: values for the *attenuation*.

ones or conservation laws which correspond to the number of macroscopic variables (in 2D, there are only four—i.e., one mass, two momenta, one energy). Thus there are unphysical

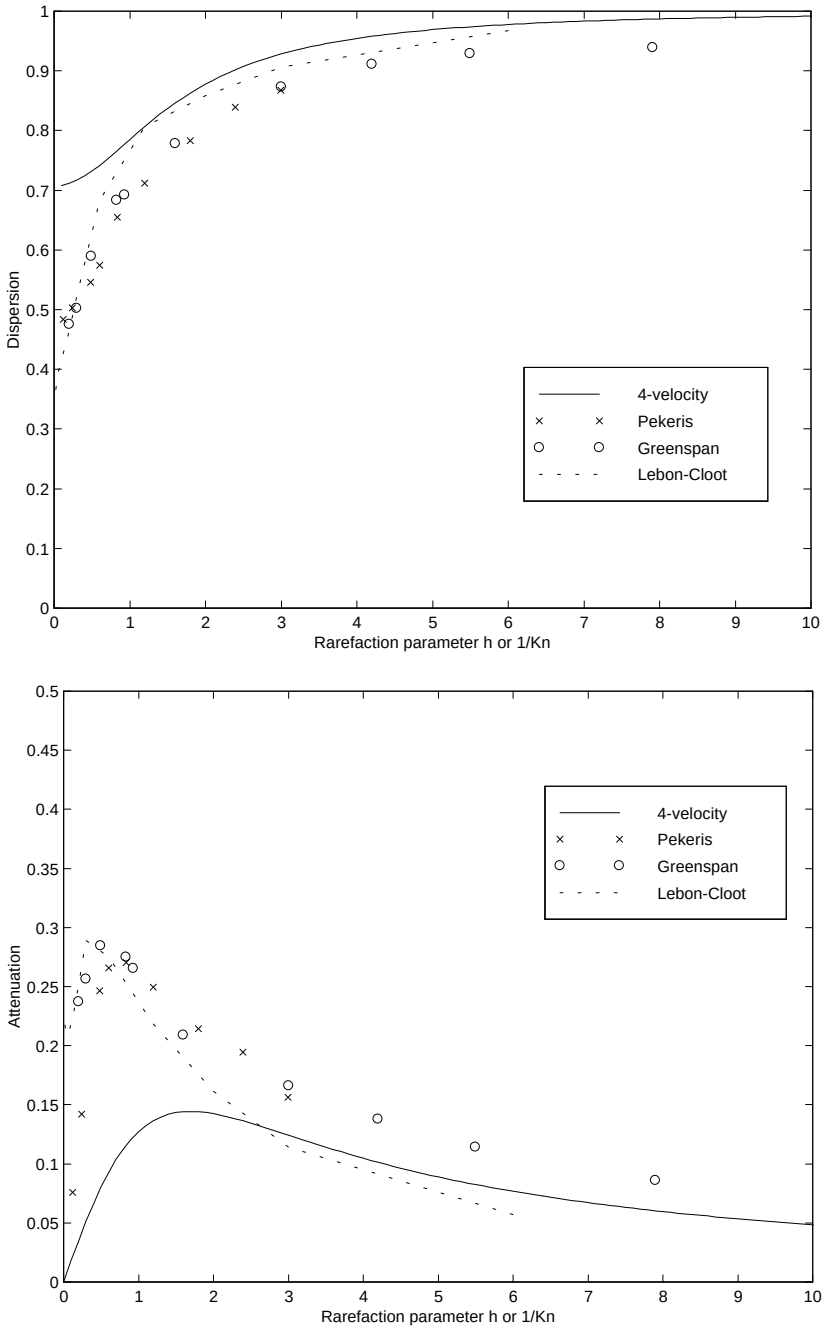

Figure 2. Comparison with Greenspan's measurements for the dispersion (upper panel) and attenuation (lower panel) with respect to the rarefaction parameter h. Calculated λ_r: values for the *dispersion*; and λ_i: values for the *attenuation*.

(spurious) invariants or macroscopic variables for $n \geqslant 3$ [21, 22] which produce the essential differences between the results of from four- and six- or eight-velocity models.

Table 1. Some of the data compared in figure 2.

h	λ	Greenspan	Four velocity	Lebon–Cloot
0.2	λ_r	0.474	0.711	0.465
	λ_i	0.237	0.035	0.251
0.3	λ_r	0.503	0.717	0.522
	λ_i	0.256	0.051	0.289
0.5	λ_r	0.588	0.732	0.66
	λ_i	0.285	0.081	0.279
0.83	λ_r	0.683	0.763	0.71
	λ_i	0.275	0.114	0.26
0.93	λ_r	0.693	0.774	0.74
	λ_i	0.266	0.121	0.246
1.60	λ_r	0.778	0.846	0.83
	λ_i	0.209	0.144	0.19
3.0	λ_r	0.873	0.928	0.906
	λ_i	0.166	0.124	0.114
4.2	λ_r	0.911	0.958	0.934
	λ_i	0.138	0.101	0.085
5.5	λ_r	0.93	0.974	0.95
	λ_i	0.114	0.082	0.08
7.9	λ_r	0.94	0.987	—
	λ_i	0.085	0.061	—

(iii) The diffusion mode [5, 14, 24–26], or the related *entropy wave*, however, may be found to have another physical meaning once relevant measurements can be conducted. Up to now, the measurements available for comparison were all from before the middle of the 1950s [11, 27].

As for the damping of the sound mode, it is seen that the absorption coefficient increases at small frequencies up to a maximum value at $h \sim 1$ and then decreases slowly for high frequencies. It was pointed out in [27] that at high values of h there may be a contribution to the absorption arising from diffusion in the piezoelectric receiver, so the experimental result for the absorption or attenuation factor should be considered as an upper limit to the actual value.

To conclude, as regards the results for the sound mode, it has been observed that, whereas the Navier–Stokes approach provides a good modelling at low frequencies, it is definitely not adequate at high frequencies with $h \leqslant 2$—especially as regards the zero dispersion (phase speed) as h approaches zero. By using the extended irreversible thermodynamics in its simplest version [11, 23], i.e., with the heat flux and the viscous pressure tensor as the only extra variables, Lebon and Cloot [23] obtained more satisfactory results for the phase speed. Unfortunately, their results for the absorption coefficient become even worse than those based on the Navier–Stokes theory as soon as $h \leqslant 1$.

Comparing with the EIT approaches [11, 23, 28] (which normally need to tune a few constants of the time relaxation), which provide another method for describing the thermal motion [29], our approach of using the four-velocity model, which is simpler than previous numerical approaches, works quite well for $h \geqslant 1.5$. Moreover, as the technique of ultrasound measurement has made progress since the early measurements of Greenspan in the middle of the 1950s [2, 3], we hope to compare the complete data (especially for the diffusion mode) from our models in the future with the newest and most reliable experimental ones, which should filter out the noise in the regime of very small h. That is because, as commented on before, earlier measurements, like those for the attenuation, in the regime of very small h, were still mixed with much unnecessary noise and many spurious fluctuations.

Meanwhile, the results from our six- and eight-velocity models can also capture well the propagation of the diffusion mode. The latter results were never derived by using the discrete kinetic theories [30] and have seldom been presented in the treatment of ultrasound propagation using continuous kinetic theories since 1965 (as reported by Mason [5]). Previous, rather complicated, analytical and numerical approaches like those of Pekeris *et al* and/or Lebon and Cloot did not produce data on the propagation of the diffusion mode.

Research interest in dilute Bose gases, e.g. equilibrium or non-equilibrium thermodynamics, has recently increased markedly and led to intensive study. Our approach, simpler and more direct than others for the treatment of hard-sphere gases, could be adapted to this new kind of problem. The results presented here, like those for the diffusion mode, might also give more clues as regards how to approach the investigation of the ultrasound propagation of dilute Bose gases. At least (perhaps not the best use), our presentation here should be useful to studies of similar or related problems in the microdomain and/or nanodomain [31].

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