Sound dispersion in single-component systems

Duncan G. Napier\textsuperscript{a}, Bernie D. Shizgal\textsuperscript{b,\ast}

\textsuperscript{a}Department of Molecular Biology and Biochemistry, Simon Fraser University, Burnaby, British Columbia V5A1S6, Canada
\textsuperscript{b}Department of Chemistry, University of British Columbia, Vancouver, British Columbia V6T1Z1, Canada

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Abstract

The present paper considers the theoretical description of the propagation of sound waves in a one component monatomic gas. The interatomic potential is assumed to vary as the inverse fourth power of the interatomic separation, that is for so-called Maxwell molecules. The eigenvalues and eigenfunctions of the linearized Boltzmann collision operator are known for this model. We emphasize the behaviour of this system in the rarefied, large Knudsen number regime for which the convergence of solutions of the Boltzmann equation can be very slow. We carry out a detailed comparison of the previous formalisms by Wang Chang and Uhlenbeck [C.S. Wang Chang, G.E. Uhlenbeck, The kinetic theory of gases, in: G.E. Uhlenbeck, De Boer, (Eds.), Studies in Statistical Mechanics, vol. 5, Elsevier, New York, 1970, pp. 43–75], Alexeev [B.V. Alexeev, Philos. Trans. R. Soc. A 349 (1994) 357] and Sirovich and Thurber [L. Sirovich, J. K. Thurber, J. Math. Phys. 10 (1969) 239]. The latter exploit a general method of solution of the Boltzmann equation developed by Gross and Jackson. We demonstrate that the Generalized Boltzmann Equation proposed by Alexeev is not appropriate and we show the reasoning for the success of the Sirovich Thurber approach over the Wang Chang and Uhlenbeck calculations. Comparisons are made with experimental data.

\textsuperscript{\ast} Corresponding author. Tel.: +1 604 82 3997; fax: +1 604 822 2847.
E-mail address: shizgal@chem.ubc.ca (B.D. Shizgal).

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1. Introduction

The kinetic theory for dispersion and absorption of sound waves in gases has a very long history [1–15]. It has attracted this ongoing interest as it is one of the most fundamental problems in kinetic theory. Methods of solution of the Boltzmann equation are required to provide accurate solutions over a very large range of Knudsen numbers from the hydrodynamic regime to the collisionless regime. The problem is related to the analogous problem dealing with light scattering from gaseous systems [16–20]. Theoretical considerations have generally considered simple monatomic gases as well as binary mixtures of inert gases [21]. There are also potential applications of similar kinetic theory treatments to polyatomic molecules [22] and also reactive systems [23]. The potential breakdown of classical Navier–Stokes treatments of transport and sound properties in and around microdevices has been raised ([24] and the references cited within). Such devices, often referred to as microelectro-mechanical systems (MEMS), are currently upwards of 1 \mu m in size and fabricated using integrated-circuit manufacturing techniques. As the mean-free path of
the gas approaches the physical dimensions of the device (that is, Knudsen number gets larger), gas kinetic treatments would be expected to yield more accurate models of these systems. Microelectro-mechanical acoustical gas sensors that measure bulk properties of gases using sound velocity measurements have been designed and constructed [25]. The concept is described in United States Patent 7146857 as an apparatus for “real time analysis of gas mixtures” [26]. Applications of these devices include environmental monitoring (air quality, humidity) and medical applications (respiratory diagnostics). The inventors’ physical models and design guidelines are currently restricted to classical fluid treatments.

The Navier–Stokes equations apply to a description of sound propagation in the limit where conventional continuum hydrodynamics holds. Experimental results obtained by Greenspan [27,28] and Meyer [29] over forty years ago demonstrated that continuum equations of hydrodynamics for small-amplitude periodic disturbances are not valid for rarefied gases and for high-frequency oscillations. The breakdown of the hydrodynamic approach occurs as the frequency of the applied oscillation approaches the collision frequency of the gas. One of the first kinetic theory treatments was by Wang Chang and Uhlenbeck (WCU) who solved the Boltzmann equation with the expansion of the velocity distribution function in a finite number of Burnett functions and reduced the Boltzmann equation for Maxwell molecules to a system of linear equations [30]. Maxwell molecules refer to particles that interact via a force law \( F(r) \sim r^{-5} \), where \( r \) is the intermolecular separation. For a solution to exist, the determinant of this set of equations must vanish, giving a dispersion relation. Successive truncations of the Burnett expansions correspond to successive terms in a power series representation of the roots of the dispersion relation [30]. The expansion parameter is the ratio of the disturbance frequency to the frequency of collisions in the gas (the Knudsen number, \( Kn \)). Comparison with experimental data shows that the WCU approach extends the validity of the dispersion relations beyond the range of continuum models but is still restricted to systems in which the frequency of the disturbance is not significantly larger than the collision frequency, that is, systems that are close to equilibrium. Pekeris and co-workers [31,32] solved the Boltzmann equation with up to 483 Burnett functions and obtained a dispersion relation. In the rarefied (Knudsen) region, \( Kn > 1 \), the results of Pekeris for the phase velocity and attenuation showed poor convergence and did not agree with experimental results, demonstrating the limitations inherent in the WCU method.

Sirovich and Thurber [2,6] proposed a model of the linearized Boltzmann collision operator that gave good agreement with experimental dispersion relations over the entire range of Knudsen number. The model used an approximation scheme proposed by Gross and Jackson [1]. Almost all work to that point describes the properties of single-component monatomic gases with Maxwell or hard sphere interatomic potentials.

Experimental results obtained by Meyer [29] show that the nondimensionalized phase velocity and attenuation rate are relatively insensitive to the interparticle potential when \( Kn \gg 1 \) owing to the low collision frequency. It has been shown that gas kinetic models with purely repulsive interparticle potentials [2,4,5] give reasonably good agreement with experimental results [27–29] over a wide range of \( Kn \). In order for a disturbance to propagate as a coherent plane wave in a gas, the disturbed particles have, on average, to collide at a higher frequency than that of the oscillation. At very high frequencies, the perturbing frequency exceeds the mean collision frequency and coherent propagation is carried mainly through the high-energy tail of the distribution function, which also accounts for the observation that sound tends to propagate at higher velocity at higher frequencies. Since high-energy collisions tend to be affected primarily by the repulsive part of the interparticle potential, this may perhaps explain the accuracy of calculations using model repulsive potentials including Maxwell molecules.

Garcia and Siewert [15] recently reported a discrete ordinate method of solution of the Boltzmann equation. The method involves the representation of the collision operator as an integral operator with the well-known kernel for hard sphere scattering. This kernel diverges for the Maxwell molecule potential (and other potentials) owing to the divergence of the classical differential cross-section at zero scattering angle [33]. The kernel is decomposed into its Legendre polynomial components and the Boltzmann equation is solved with a numerical quadrature and subject to a boundary condition analogous to other half-space problems in kinetic theory. The number of Legendre components and quadrature points required to achieve convergence is large, and thus the computational costs of the method are considerable. They report generally good agreement with experiment except in the large Knudsen number regime attributed in part to the treatment of the problem as a half-space problem subject to a boundary condition. The discrete ordinate method does not permit the analytic analysis that we present in this paper based on moment methods that can provide exact results in the near hydrodynamic limit.

In the following sections, the reasons for the failure of the WCU method at high frequencies/low pressures are examined, together with proposed solutions to the breakdown of the WCU method. The recent theory of Alexeev [13,14]
based on the GBE is examined along with the much earlier work of Sirovich and Thurber [2,6,7]. The purpose of this work is to understand the behaviour of sound waves at high frequencies and low pressures, and in other cases where hydrodynamic theories are no longer valid. The anomalous sound dispersion behaviour observed experimentally in mixtures of gases near the intermediate zone between the hydrodynamic and collisionless regions has been reported elsewhere [19,20].

2. Boltzmann equation for small-amplitude disturbance

The time-evolution of the velocity distribution function of a gas in the absence of external forces is

$$\left( \frac{\partial}{\partial t} + \mathbf{c} \cdot \nabla \right) f = J[f]$$

(1)

where $J[f]$ is the Boltzmann collision integral

$$J[f] = \int \int [f_{i} - f_{i}] \sigma g d\Omega d\epsilon_{1}$$

(2)

and $\sigma(g, \Omega)$ is the differential collision cross-section which depends on the magnitude of the relative velocity, $g = c - c_{i}$, and the scattering angle $\Omega$.

If an oscillation is applied to the gas, the velocity distribution function departs from the Maxwellian by a small term so that,

$$f(c, r, t) = f^{(0)}(c)[1 + h(c, r, t)].$$

(3)

If Eq. (3) is substituted into Eq. (1) and only linear terms in $h$ are taken, followed by use of the identity $f^{(0)\prime} f^{(0)\prime} = f^{(0)} f^{(0)}$, it is found that the linearized Boltzmann equation is of the form

$$\left( \frac{\partial}{\partial t} + \mathbf{c} \cdot \nabla \right) h = \kappa K[h]$$

(4)

where $K$ is a nondimensional form of the linearized Boltzmann collision operator and

$$K[h] = \frac{1}{\kappa} \int \int f^{(0)}[h(c') + h_{1}(c_{1}') - h(c) - h_{1}(c_{1})] g d\Omega d\epsilon_{1}.$$  

(5)

The dimensionless time variable $\kappa t = t (\frac{2kT}{\sigma_{0}})^{1/2}$ scales inversely with the mean-free path $l = 1/n\sigma_{0}$, where $\sigma_{0}$ is some constant cross-section of the order of magnitude of the collision cross-section.

A pressure fluctuation propagates as a plane wave (normal mode) in the ideal fluid approximation [34] and the perturbation $h$ is written as

$$h(c, r, t) = h(c) e^{i(k \cdot r - \omega t)}$$

(6)

where the wave vector $k = \hat{k}|k|$ defines the direction of propagation, and the frequency of the oscillation is $\omega$. With Eq. (6) and the $x$-axis of the space coordinate, $r$, along $\hat{k}$, Eq. (5) is now

$$(E - \epsilon \xi) h = K[h]$$

(7)

where $E = -i(\frac{m}{2kT})^{1/2}\omega = -i\omega/\kappa$, $\epsilon = -ikl$, $\xi = (\frac{m}{2kT})^{1/2}c$, and $\kappa \xi = \hat{k} \xi$. We consider alternate methods of solution of the linearized Boltzmann equation, Eq. (7), in the sections that follow.

2.1. The method of Wang Chang and Uhlenbeck

The disturbance is a plane wave propagating in direction $k$, taken to lie along the polar axis $x$. The perturbation $h$ is written as an expansion in the axially-symmetric Burnett functions $\psi_{nl}(\xi, \theta)$,

$$h(\xi, \theta) = \sum_{n,l=0}^{\infty} a_{nl} \psi_{nl}(\xi, \theta)$$

(8)
where \( \theta \) is the angle between \( \xi \) and the polar axis and

\[
\psi_{nl}(\xi, \theta) = N_{nl} \xi^l L_n^{l+1/2}(\xi^2) P_l(\cos \theta).
\] (9)

The Legendre polynomials, \( P_l(\cos \theta) \) and associated Laguerre polynomials, \( L_n^{l+1/2}(\xi^2) \), have their usual definitions [35–37]. The basis functions \( \psi_{nl} \) are normalized according to

\[
\langle \psi_{nl}, \psi_{n'l'} \rangle = \int e^{-\xi^2} \psi_{nl}(\xi) \psi_{n'l'}(\xi) d\xi = \delta_{nn'} \delta_{ll'}.
\] (10)

Eq. (7) is solved by substituting the expansion Eq. (8), multiplying by each basis function and integrating over \( \xi \). The result is a set of simultaneous linear equations in \( a_{nl} \) written in matrix notation

\[
(EI - \epsilon C - K)a = 0.
\] (11)

The matrix \( I \) is the identity matrix, and the elements of \( C \) and \( K \) are explicitly

\[
C_{nl,n'l'} = \langle \psi_{n'l'}, \xi_n \psi_{nl} \rangle
= \pi^{-3/2} \int_{-\infty}^{\infty} e^{-\xi^2} \psi_{nl}(\xi) \xi_n d\xi
\] (12)

and

\[
K_{nl,n'l'} = \langle \psi_{nl}, K[\psi_{n'l'}] \rangle
= \pi^{-3/2} \int \int \int e^{-\xi^2-\xi'^2} \psi_{nl}(\xi_1) \psi_{n'l'}(\xi_1') \psi_{n'l'}(\xi_2') \psi_{n'l'}(\xi_2) \sigma \Omega d\xi_1 d\xi_2.
\] (13)

For Maxwell molecules, the axially-symmetric Burnett functions, \( \psi_{nl} \) in Eq. (9), are eigenfunctions of the collision operator \( K \). For this special case,

\[
K_{nl,n'l'} = \lambda_{nl} \delta_{nn'} \delta_{ll'}
\]

where \( \lambda_{nl} \) are the eigenvalues of collision operator, \( K \) are known [36]. The integral expression \( \lambda_{nl} \) was evaluated by Gaussian Legendre quadrature. Tables of \( \lambda_{nl} \) are also available [32]. In particular, \( \lambda_{00} = \lambda_{01} = \lambda_{10} = 0 \).

The matrix elements of \( C \) defined by Eq. (12) are given explicitly by

\[
C_{nl,n'l'} = (l + 1) \left( \frac{n + l + \frac{3}{2}}{(2l + 3)(2l + 1)} \right)^{1/2} \delta_{nn'} \delta_{(l+1)l'} - (l + 1) \left( \frac{n}{(2l + 3)(2l + 1)} \right)^{1/2} \delta_{(n-1)n'} \delta_{(l+1)l'}
+ l \left( \frac{n + l + \frac{1}{2}}{(2l + 1)(2l - 1)} \right)^{1/2} \delta_{nn'} \delta_{(l-1)l'} - l \left( \frac{n + l}{(2l + 1)(2l - 1)} \right)^{1/2} \delta_{(n+1)n'} \delta_{(l-1)l'},
\] (14)

where we have used the recurrence relation [35] in terms of \( \psi_{nl} \) which can be inferred from Eq. (14).
2.2. Sound dispersion relations

The dispersion relation that is sought relates the phase velocity and attenuation of a disturbance to its frequency. The form of the dispersion relation depends on whether the oscillations are free or forced. We take the x-axis to be the direction of propagation so that the wave number is \( k = \beta + i\alpha \) and the space and time-dependence of the perturbation in Eq. (6) is given by \( e^{i(kx - \omega t)} = e^{-\alpha x + i(\beta x - \omega t)} \). Forced oscillations decay over distance, and the wave number, \( k \) is a complex number for which the real component \( \beta \) corresponds to the phase of the wave and the imaginary component \( \alpha \) corresponds to the attenuation (\( \beta \) and \( \alpha \) are real and positive). The applied frequency \( \omega \) is real. For forced normal-mode oscillations we have that \( \text{Im}[k] = \alpha \geq 0 \) and \( v = \omega/\text{Re}[k] = \omega/\beta \) where \( v \) is the propagation or phase velocity of the normal mode. Free oscillations, on the other hand, decay over time and in this case, \( \omega = \beta + i\alpha \) where the perturbation is now given by \( e^{i(kx - \omega t)} = e^{i\alpha t + i(\beta x - \beta t)} \) where \( \text{Im}[\omega] = \alpha \leq 0 \), and \( v = \text{Re}[\omega]/k = \beta/k \).

2.3. Solution of dispersion relations for the WCU method

A solution for the system of homogeneous equations, Eq. (11) exists only when the secular determinant vanishes,

\[
|EI - \epsilon C - K| = 0. \tag{15}
\]

The determinant Eq. (15) yields the dispersion relation for the system. Phase velocities and attenuation constants at a given frequency or wavelength disturbance are computed from the roots of Eq. (15). The dispersion relation obtained from Eq. (15) can often be computed numerically with greater efficiency [38] by solving the eigenvalue problem corresponding to Eq. (11), which for the case of free sound is

\[
D(\epsilon)a = E(\epsilon)a \tag{16}
\]

where \( D(\epsilon) = \epsilon C + K \). The eigenvalues \( E(\epsilon) \), are transformed into the dimensionless form of the dispersion relation \( \omega(k) \), using the relations \( E = -i\omega/\kappa \) and \( \epsilon = -ikL \). The real and imaginary parts of \( \omega \) give the wave phase and attenuation, respectively, as a function of the wave number \( k \).

The eigenvalue matrix for forced sound is obtained by multiplying Eq. (11) by \( C^{-1} \) giving

\[
F(E)a = \epsilon(E)a \tag{17}
\]

with \( F = (EI - K)C^{-1} \). If we apply the transformations \( E = -i\omega/\kappa \) and \( \epsilon = -ikL \) we compute the eigenvalues \( \epsilon(E) \) for forced sound modes \( k(\omega) \). The real and imaginary parts of \( \omega \) are the phase and attenuation, respectively, of the wave given as a function of frequency, \( \omega \). This method was exploited by Pekeris [31] for solution of the WCU dispersion relations with up to 483 terms in Eq. (8).

Successive truncations of the matrix Eq. (11) to \((N + 1) \times (L + 1)\) terms gives a dispersion relation in power series expansions in \( \epsilon \) [30]. Wang Chang and Uhlenbeck demonstrated that for the special case of Maxwell molecules, successive approximations obtained by adding new terms merely add higher-order terms in \( \epsilon \) in the power series expansion [30]. This was demonstrated with specific examples for 3-, 5- and 8-term series solutions. The 3-term truncation uses the Burnett functions \( \psi_{00}, \psi_{01} \) and \( \psi_{10} \). The addition of the polynomials \( \psi_{02} \) and \( \psi_{11} \) corresponds to a 5-term truncation and the further addition of the polynomials \( \psi_{03}, \psi_{20} \) and \( \psi_{12} \) gives the 8-term truncation. The choice of these polynomials corresponds respectively to the Euler, Navier–Stokes and Burnett approximations to hydrodynamics. Wang Chang and Uhlenbeck note that the power-law dependence in \( \epsilon \) of the dispersion relation can be proven for all cases and arises from the selection rule of the matrix \( C \) of Eq. (14), which is \( C_{nl,n'l'} = 0 \), unless \( 2n' + l' = 2n + l \pm 1 \). The selection rule ensures a band-diagonal matrix that does not extend farther from the diagonal as one adds more elements in going from an \( n \)th-order approximation to an \((n + 1)\)th-order approximation. Ford and Foch [34] showed that each new term in the series added higher-order terms to the hydrodynamic dispersion relation and noted that the dispersion law would be unsuitable for cases where the ratio of the mean-free path to wavelength was large. Results obtained with the WCU method are shown in the next section. We reproduce data from earlier work [31,34] in order to confirm the results and corroborate the conclusions of these studies as well as to provide a basis for comparison with other approaches. This discussion is deferred to later sections.
2.4. Solutions with the WCU method

For the case of forced sound studied by Greenspan and Meyer [27–29], the frequency of oscillation, $\omega$, is real and the wave number takes a complex value of the form $k = \beta + i\alpha$ where $\beta$ is the phase and $\alpha$ is the attenuation. In the physical situation addressed, $\alpha \geq 0$. The ratio $\alpha/\omega$ is termed the attenuation rate by Greenspan [27,28] and $\omega/\beta$ is the phase velocity of the plane wave. Changes in phase velocity and attenuation with frequency are presented in the dimensionless forms $\alpha v_0/\omega$ and $\beta v_0/\omega$, respectively. Calculations for the simplest case, that of Maxwell molecules, are presented.

The lowest-order WCU matrix is the set of equations that conserve mass, momentum and energy and corresponds to the Euler approximation to hydrodynamics. The perturbation is written in the form

$$h = a_{00}\psi_{00} + a_{01}\psi_{01} + a_{10}\psi_{10}$$  \hspace{1cm} (18)

with only the eigenfunctions of the linearized collision operator $K$ having zero eigenvalues.

Consequently, the collision term $K[h]$ in Eq. (11) vanishes and the secular determinant gives,

$$E \left( E^2 - \frac{5}{6} \epsilon^2 \right) = 0$$ \hspace{1cm} (19)

with three solutions, $E = 0$ and $\frac{\epsilon}{E} = \pm \sqrt{\frac{6}{5}}$. The solution $E = 0$ is spurious since the applied frequency is not identically zero. The $\frac{\epsilon}{E}$ term can be written as an expression in $k$ and $\omega$ using the results $E = (\frac{m}{2k_BT})^{1/2} \omega$ and $\epsilon = -i kl$ to give

$$\frac{\omega}{\beta} = \pm \sqrt{\frac{5}{6}} \frac{2k_BT}{m}$$ \hspace{1cm} (20)

which is consistent with the adiabatic speed of sound for an ideal gas, $\gamma = 5/3$. In the Euler approximation there is no dissipation and therefore no damping term, resulting in $\alpha \equiv 0$.

Analogously, the 4-term expansion for the WCU method involves the addition of $\psi_{11}$ to the expansion. With $K_{11,11} = \lambda_{11} = -2/5$, the secular determinant of the $4 \times 4$ matrix Eq. (11), is after division by $E^4$

$$1 + \frac{2}{5} \frac{1}{E} - \frac{5}{3} \left( \frac{\epsilon}{E} \right)^2 - \frac{1}{3} \left( \frac{\epsilon}{E} \right)^2 \frac{1}{E} + \frac{1}{3} \left( \frac{\epsilon}{E} \right)^4 = 0.$$ \hspace{1cm} (21)

The term $\frac{\epsilon}{E}$ is a dimensionless complex number of magnitude

$$\left| \frac{\epsilon}{E} \right| = \sqrt{\left( \frac{\beta}{\omega} \right)^2 + \left( \frac{\alpha}{\omega} \right)^2 \frac{2k_BT}{m}}$$ \hspace{1cm} (22)

($\alpha$, $\beta$ and $\omega$ are real) where $\beta/\omega$ and $\alpha/\omega$ are the reciprocals of the phase velocity and the attenuation coefficient, respectively. The hydrodynamic limit is the limit of low frequencies, $\omega \to 0$ or $1/E \to \infty$. The quantity $\epsilon/E$ goes to a constant in the asymptotic limit $\omega \to 0$ consistent with the phase velocity and attenuation rate in the hydrodynamic limit. Eq. (21) in this limit is

$$\frac{2}{5} - \frac{1}{3} \left( \frac{\epsilon}{E} \right)^2 = 0$$ \hspace{1cm} (23)

which gives the phase velocity $\frac{\omega}{\beta} = \pm \sqrt{\frac{5}{6}} \frac{2k_BT}{m}$ consistent with the results for an ideal gas. Eq. (23) also gives the correct attenuation factor in the hydrodynamic limit $\frac{\alpha}{\omega} = 0$, which is also consistent with the Euler approximation to hydrodynamics.

The Knudsen limit is $\omega \to \infty$ or $1/E \to 0$. The quantity $\epsilon/E$ goes to a constant in this limit, as shown by experimental results [27,28], and Eq. (21) becomes

$$\frac{1}{3} \left( \frac{\epsilon}{E} \right)^4 - \frac{5}{3} \left( \frac{\epsilon}{E} \right)^2 + 1 = 0$$ \hspace{1cm} (24)
Fig. 1. Log–log plot of WCU method results for (A) $\beta \omega^{-1} v_0$ and (B) $\alpha \omega^{-1} v_0$ versus $1/Kn$. The number of moments retained are 4, 6, 16, 20 and 36, NS is the Navier–Stokes result and experimental results are denoted by $\circ$.

and the dispersion relation in the limit of large applied frequencies is

$$
\frac{\beta v_0}{\omega} = \pm \sqrt{2 \left( 1 \pm \sqrt{\frac{2}{5}} \right) \sqrt{\gamma}}
$$

$$
\frac{\alpha v_0}{\omega} = 0.
$$

(25)

The phase velocity of sound at high frequencies is typically greater than that at low frequencies, and $\beta v_0/\omega < 1$. This is attributed to the fact that slower-moving particles are less able to transmit a high-frequency disturbance. The fastest-moving particles tend to have higher collision frequencies and are able to transmit the disturbance more effectively. This leads to the choice of the conjugate pair of solutions from Eq. (25) $\lim_{\omega \to \infty} \frac{\beta v_0}{\omega} \sim \pm 0.7826$ as the 4-term approximation to the phase velocity in the Knudsen limit. This agrees qualitatively with experimental results [27–29] which show that the phase velocity of a gas increases to a fixed asymptotic limit ($|\beta v_0/\omega| \sim 0.5$) in the Knudsen region.

Higher-order dispersion relations were obtained by successive truncations to the WCU matrix. The matrix equation Eq. (11) was truncated at $n' = N$ and $l' = L$ and the phase velocity and attenuation as well as the numerical convergence was studied. The zeroes of Eq. (15) were computed numerically for successively higher-order truncations using the Newton–Raphson method. The numerical double-precision “zero of the polynomial” was less than $10^{-15}$ on substitution of the final Newton–Raphson iterate into the polynomial. The results from the root-searching were checked for consistency by cross-comparison with results obtained from the numerical solution of the eigenvalue problem Eq. (17).

The zeroes of the secular determinant for forced sound gave $k(\omega)$. The real part of $k$ corresponds to $\beta$, the phase, and the imaginary part of $k$ is $\alpha$, which corresponds to the attenuation. The phase velocity, $\omega/\alpha$, and attenuation rate, $\beta/\omega$, obtained for a series of $N$ and $L$ truncations and the results were compared with those from experiment [27–29]. Matrix truncations of higher order than the Euler approximation result in dispersion relations with more solutions than there are sound modes. For systems with multiple roots, the sound modes were identified by their low-frequency behaviour: as $\omega \to 0$, $\omega/\beta$ (corresponding to the hydrodynamic phase velocity) goes to a known positive constant while $\alpha/\omega$ (the hydrodynamic attenuation rate) goes to zero.

Fig. 1A shows $\beta \omega^{-1} v_0$, the reciprocal of the dimensionless phase velocity, plotted against $1/Kn$ for a series of successive truncations. The numeric labels on the curves correspond to the number of Burnett functions retained in the WCU matrix. The 4-term expansion is truncated at $R = 1, L = 1$, the 6-term is truncated at $R = 2, L = 1$, 16-term at $R = 3, L = 3$, 20-term at $R = 4, L = 3$ and 36-term at $R = 5, L = 5$. The Navier–Stokes result from conventional hydrodynamics fails to reproduce the experimental result and is shown by a dashed line labeled NS. Phase velocities obtained with the WCU method converge quickly in the limit of small $Kn$ and coincide with the hydrodynamic result ($\beta \omega^{-1} v_0 = 1$) for this limit. The phase velocity becomes larger than the hydrodynamic phase
velocity around $1/Kn < 10$, and reaches its asymptotic value that varies between 0.8 and 0.5 for $Kn \sim 1$ in the Knudsen region. The results agree qualitatively with experimental results for argon (circles on Fig. 1A) but even with 36 terms, still do not appear to converge. Pekeris reports convergence using 483 terms [31].

The corresponding attenuation rates are shown in Fig. 1B. The 3-term or Euler approximation (not plotted here) predicts no attenuation. The 4-term approximation ($N = 1, L = 1$, Eq. (21)) of the WCU method gives attenuation rates that are significantly smaller than all higher-order approximations (curves labeled 6, 16, 20 and 36 in Fig. 1B). This behaviour is consistent with the hydrodynamic interpretation of the effect of higher-order terms. The moments used in the 4-term approximation are $\psi_{00}, \psi_{01}, \psi_{10}$ and $\psi_{11}$ which correspond to mass, velocity, energy and heat flux. The 4-term solution gives the behaviour of sound in a thermally conducting, frictionless gas. The influence of heat conduction and viscosity are of the same order of magnitude and therefore both must be accounted for by a consistent solution. (The Prandtl number measures the importance of viscosity and heat conductivity and has been found experimentally to be of order unity for all gases). The 4-term solution is analogous to early treatments of sound propagation (Stokes, c. 1845) that included the effect of viscosity (which corresponds to the next highest moment, $\psi_{02}$) but not heat conduction. Lamb [39] obtained a hydrodynamic solution for the case involving both viscosity and heat conduction and the results showed that sound waves in that case are more strongly attenuated than when one of the effects is neglected. Lamb’s results also showed that the hydrodynamic propagation velocity remained virtually unaffected by the influence of dissipative effects. These results are consistent with 6-term and higher-order WCU results for the hydrodynamic region (curves 6, 16, 20, and 36). The phase velocity in the hydrodynamic region is unaffected by higher moments and virtually all attenuation in the hydrodynamic region arises from low-order moments (that, is heat conduction and viscosity).

All attenuation rates obtained for 5-term and higher-order truncations coincide with the Navier–Stokes result (dashed line) in the hydrodynamic limit. The attenuation rates obtained from the WCU method show poor agreement and poor convergence with experimental results for $Kn > 1$. The WCU method predicts that the attenuation rate for sound vanishes as in the limit of large $Kn$, while experimental results show that the attenuation rate approaches constant value $\approx 0.22$ in that limit.

### 2.5. The generalized Boltzmann equation (GBE) method of Alexeev

Alexeev [13,14] proposed a GBE which has been claimed to be valid over all $Kn$. The method of Alexeev is in sharp contrast to the efforts of other workers who proposed approximate solutions based on various treatments of the collision operator [2–4]. Alexeev has suggested that the difficulty with the solutions of the Boltzmann equation in the collisionless limit, $Kn \to \infty$, lies not with the method of solution of the Boltzmann equation but with the Boltzmann equation itself [13,14]. Alexeev has attempted to solve the problem of sound dispersion at high frequencies and low pressures by rewriting the LHS of the Boltzmann equation, Eq. (1).

The time-evolution of the velocity distribution function of a gas in the absence of external forces is typically written [37]

$$\frac{Df}{Dt} = J[f] \tag{26}$$

where $J[f]$ is the Boltzmann collision integral, Eq. (2). Alexeev has proposed instead writing Eq. (26) as

$$\frac{Df}{Dt} - \tau \frac{D}{Dt} \frac{Df}{Dt} = J[f] \tag{27}$$

where $\tau$ is the mean-free time between collisions.

The linearized form of the GBE follows from the linearization of $J[f]$ in Section 2 and is

$$\left(\frac{D}{Dt} - \tau \frac{D}{Dt} \frac{D}{Dt}\right) h = \kappa K[h]. \tag{28}$$

A periodic perturbation $h$ of the form Eq. (6) is substituted into Eq. (31) in the manner of the WCU giving the linearized GBE

$$\left[(E - \epsilon \xi_x) - \frac{1}{\nu} (E - \epsilon \xi_x)^2\right] h = K[h] \tag{29}$$
where the nondimensionalized collision frequency is \( \nu = \frac{1}{\kappa} \). The behaviour of sound as described by the GBE is obtained solving Eq. (29) for the dispersion relation.

Alexeev has presented the generalized hydrodynamic solution which he has suggested extends hydrodynamic theory past the intermediate region and into the Knudsen region [13]. Alexeev called these new hydrodynamical equations the generalized hydrodynamic equations. These generalized hydrodynamic equations are 3- and 5-term approximations to the generalized Boltzmann equation, which Alexeev has called the generalized Euler and generalized Navier–Stokes equations, respectively [13]. Presented here is the solution to Alexeev’s GBE, which, if consistent to all orders in \( h \), should address the failure of the WCU solution to agree with experimental results over all \( Kn \).

As was done in the previous sections, Eq. (29) is solved by substituting the expansion Eq. (8), multiplying by each basis function and integrating over \( \xi \). The result is a set of simultaneous linear equations in \( a_{nl} \). The generalized Boltzmann approach gives the matrix equation

\[
\left[ EI - \gamma_1 (\epsilon C + K) - \gamma_2 \frac{\epsilon^2}{\nu} D \right] a = 0
\]

where \( \gamma_1 = \frac{2E/\nu - 1}{E/\nu - 1} \) and \( \gamma_2 = \frac{1}{(1-E/\nu)} \) and the elements of \( C \) and \( K \) are defined in Eqs. (12) and (13), respectively. The elements of the matrix \( D \),

\[
D_{nl,n'l'} = (\psi_{nl}, \xi^2 \psi_{n'l'})
\]

are obtained in an analogous manner to the calculation of \( C_{nl,n'l'} \) by using the recurrence relation for \( \xi, \psi_{nl} \) twice in an obvious manner. The resulting expression, which consists of sixteen terms, can be found elsewhere [35]. The zeroes of the determinant for the system of homogeneous equations yield Eq. (30), a dispersion relation for \( E \) in terms of \( \epsilon \).

### 2.6. Comparison of WCU and GBE methods

The matrix representation of the GBE, Eq. (30), can be truncated at 3-terms to give the Euler approximation to generalized hydrodynamics. With the explicit values of the \( 3 \times 3 \) matrices, \( C, K \) and \( D \) we find that,

\[
\gamma_1 (\epsilon C + K) + \gamma_2 \frac{\epsilon^2}{\nu} D = \begin{pmatrix}
\gamma_2 \frac{\epsilon^2}{2 \nu} & \gamma_1 \sqrt{\frac{1}{2} \epsilon} & \gamma_2 \sqrt{\frac{1}{6} \epsilon} \\
\gamma_1 \sqrt{\frac{1}{2} \epsilon} & \frac{7 \epsilon^2}{6 \nu} & \gamma_1 \sqrt{\frac{1}{3} \epsilon} \\
\gamma_2 \sqrt{\frac{1}{6} \epsilon} & \gamma_1 \sqrt{\frac{1}{3} \epsilon} & \gamma_2 \frac{3 \epsilon^2}{2 \nu}
\end{pmatrix}
\]

The dependence of the dispersion relation upon the Knudsen number, \( Kn \), was of particular interest. For the case of the GBE, \( Kn \) appears explicitly in the dispersion relation. Since \( Kn = |E/\nu| \), the dispersion relation of the linearized GBE for \( E \neq 0 \), to lowest order, can be written as a 6th-order polynomial in \( E/\epsilon \) by dividing by \( E^3 \) giving

\[
\left[ EI - \gamma_1 (\epsilon C + K) - \gamma_2 \frac{\epsilon^2}{\nu} D \right] = i \left( \frac{1}{Kn} \right)^3 - \frac{1}{Kn} \frac{5}{6} \frac{\epsilon^2}{E^2} \left( \frac{1}{Kn} \right)^3 \\
+ \frac{5}{12} \frac{\epsilon^4}{E^4} \left( \frac{1}{Kn} \right)^2 + \frac{\epsilon^2}{E^2} \left( \frac{1}{Kn} \right)^2 - 3i \left( \frac{1}{Kn} \right) \\
- \frac{5}{3} \frac{\epsilon^4}{E^4} \left( \frac{1}{Kn} \right)^2 + \frac{1}{3} \frac{\epsilon^2}{E^2} \left( \frac{1}{Kn} \right)^2 - \frac{1}{6} \frac{\epsilon^2}{E^2} \\
+ \frac{5}{4} \frac{\epsilon^4}{E^4} + \frac{5}{8} \frac{\epsilon^6}{E^6} + 1
\]

\[
= 0.
\]

The GBE is reported to describe the phenomena over the full range of Knudsen number and therefore the asymptotic properties of the dispersion relation Eq. (33) are of interest. The limit of hydrodynamic limit \( Kn \rightarrow 0 \) was discussed
in the analysis of the WCU method above. The Knudsen region, for which $Kn \to \infty$ is conveniently treated using the form of Eq. (33).

In the limit $Kn \to \infty$, Eq. (33) is a cubic equation in $X = (\epsilon/E)^2$

$$\frac{5}{8} X^3 + \frac{5}{4} X^2 - \frac{1}{6} X + 1 = 0$$

(34)

with roots

$$X = A + B - \frac{2}{3}$$

(35)

$$X = \pm \frac{\sqrt{3}}{2} (A - B)i - \frac{1}{2} \left( A + B + \frac{4}{3} \right)$$

(36)

where $A = -0.40377$ and $B = -1.3209$. Collecting real and imaginary components of Eqs. (35) and (36), and taking $\alpha$ and $\beta$ to be both real, explicit values for the nondimensionalized phase velocity, $\beta v_0/\omega$ and attenuation rate $\alpha v_0/\omega$ were obtained. Eq. (35) gives a nonpropagating mode

$$\frac{\alpha v_0}{\omega} = \pm \sqrt{\frac{2}{3} - A - B} \sqrt{\frac{\gamma}{2}}$$

(37)

$$\frac{\beta v_0}{\omega} = 0.$$  

(38)

Nonpropagating modes also appear in hydrodynamic treatments, where they are known as heat conduction modes [30]. Since $\alpha \geq 0$, the growing or amplified mode $\alpha < 0$ is considered spurious and $\gamma$ is set to $5/3$ giving $\lim_{Kn \to \infty} \alpha v_0/\omega \sim 1.4117$. If we collect real and imaginary parts of Eq. (36), we find that,

$$\frac{\beta^2 - \alpha^2}{\omega^2} v_0^2 = -\frac{1}{2} \left( \frac{4}{3} + A + B \right) \frac{\gamma}{2}$$

(39)

and

$$\frac{\alpha \beta v_0^2}{\omega^2} = \pm \frac{\sqrt{3}}{4} (A - B) \frac{\gamma}{2}.$$  

(40)

The square of Eq. (40) is

$$\frac{\alpha^2 v_0^2}{\omega^2} = \left( \frac{\omega}{\beta v_0} \right)^2 \frac{3}{64} (A - B)^2 \gamma^2.$$  

(41)

With Eq. (41) substituted into Eq. (39), a quadratic in terms of the square of the phase velocity is obtained,

$$\left( \frac{\omega}{\beta v_0} \right)^4 + C \left( \frac{\omega}{\beta v_0} \right)^2 - D = 0$$

(42)

where $C = (A + B + 4/3) \gamma/4 = -0.1631$ and $D = 3(A - B)^2 \gamma^2/64 = 0.1095$. The result is a conjugated pair of roots that ultimately give rise to four solutions for the phase velocity

$$\frac{\beta v_0}{\omega} = \pm \left( \frac{C \pm \sqrt{C^2 + 4D}}{2} \right)^{1/2}$$

(43)

for the case of an ideal gas $\gamma = 5/3$. Two of the roots are spurious since they give imaginary phase velocities. The remaining two roots give the asymptotic phase velocity $\lim_{Kn \to \infty} \frac{\beta v_0}{\omega} \approx \pm 0.650$. The corresponding attenuation rate is $\frac{\alpha v_0}{\omega} = \frac{\omega}{\beta v_0} \sqrt{D}$ where for an ideal gas $\lim_{Kn \to \infty} \frac{\alpha v_0}{\omega} \approx 0.509$. The above treatment agrees with the generalized Euler equation [13], for which Alexeev also reports $\beta v_0/\omega = 0.650$ and $\alpha v_0/\omega = 0.509$ in the limit $Kn \to \infty$. The Euler approximation to the GBE gives attenuation rates that only agree qualitatively with the experimental results of Meyer for the case of greatest rarefaction, where $\beta v_0/\omega \approx 0.45$ and $\alpha v_0/\omega \approx 0.22$.  

4117.
Fig. 2. Log–log plot of GBE method results for (A) $\beta \omega^{-1} v_0$ and (B) $\alpha \omega^{-1} v_0$ versus $1/Kn$. The number of moments retained are 4, 5, 6, 16, 20 and 36 and experimental results are denoted by $\circ$. 

Fig. 2A plots $\beta \omega^{-1} v_0$ versus $1/Kn$, obtained from the dispersion relation for the GBE Eq. (69) with 3-, 4-, 5-, 20- and 36-terms. Experimental results are shown with circles. All results converge to the hydrodynamic phase velocity for large $Kn$. In the Knudsen region, the result does not appear to converge and as more terms are added to the matrix, the solutions appear to become unstable and no longer agree with the experiment. The solutions obtained by using 3-, 5- and 6-terms agree qualitatively with experimental results (circles). Fig. 2B shows a plot of $\alpha \omega^{-1} v_0$ versus $1/Kn$ for a series of successive truncations of the GBE. As with the result for phase velocities in Fig. 2A, the low-order (3-, 5- and 6-term) solutions for attenuation rates in Fig. 2B show only qualitative agreement with experiment in the asymptotic limit $1/Kn \rightarrow 0$. As more terms are added the solutions of the GBE appear to converge only slowly in the hydrodynamic region and diverge in the Knudsen region as shown in Fig. 2A and B. The WCU method fails in the Knudsen region but is consistent with experimental results and conventional hydrodynamic behaviour in the hydrodynamic region $Kn \ll 1$. These findings do not support Alexeev’s claim that the GBE-derived Generalized Hydrodynamic Equation (GHE) represents an interpolation of hydrodynamical solutions into the collisionless region. This work suggests that the GHE results presented by Alexeev appear to be unconverged series solutions of the GBE. When carried to high orders, the GBE suffers the same defects as WCU, namely nonphysical behaviour and poor convergence. It is concluded that the GBE fails to describe sound propagation behaviour over the entire range of Knudsen number.

2.7. The Sirovich–Thurber (ST) method

Citing convergence problems and obvious discrepancies between theoretical and experimental results [31,40], Sirovich and Thurber long ago proposed abandoning the WCU method in favor of a model of the linearized Boltzmann collision operator suggested by Gross and Jackson [2,6]. We briefly summarize the ST method and note in Table 1 some differences in the notation used in this paper.

When Eq. (8) is substituted into the RHS of Eq. (1), the result is

$$ (E - \epsilon \xi) h(\xi, \theta) = K[h] = \sum_{n,l,n',l'=0} a_{nl} K_{nl,n'l'} \psi_{n'l'} $$

where $K_{nl,n'l'}$ is defined in Eq. (13). Instead of the usual truncation of Eq. (44) at $N$ and $L$, Gross and Jackson [1] suggested that a more accurate approximation of the Boltzmann collision operator, Eq. (44), is

$$ K^{(GJ)}[h] = \sum_{n,l,n',l'=0}^{N,L} a_{nl} K_{nl,n'l'} \psi_{n'l'} + \lambda \sum_{n,l>N,L}^{\infty} a_{nl} \psi_{nl} $$
where $\lambda$ is some constant that approximately preserves the remainder of the collision term and a useful choice might be $\lambda_{N+1,L+1}$. Eq. (45) is transformed by adding

$$0 = \lambda \sum_{n,l=0}^{N,L} a_{nl} \psi_{nl} - \lambda \sum_{n,l=0}^{N,L} a_{nl} \psi_{nl}$$

(46)

giving

$$(E - \epsilon \xi_x - \lambda) \hbar = \sum_{n,l,n',l'=0}^{N,L} a_{nl}(K_{nl,n'l'} - \lambda \delta_{nn'} \delta_{ll'}) \psi_{n'l'}.$$  (47)

An essential aspect of the method of Sirovich and Thurber is to factor out $\epsilon$ from the LHS of Eq. (47)

$$\epsilon \left( \frac{E - \lambda}{\epsilon} - \xi_x \right) \hbar = \sum_{n,l,n',l'=0}^{N,L} a_{nl}(K_{nl,n'l'} - \lambda \delta_{nn'} \delta_{ll'}) \psi_{n'l'}$$

(48)

and then divide by the velocity-dependent term in brackets giving

$$-\epsilon \hbar = \sum_{n,l,n',l'=0}^{N,L} a_{nl}(K_{nl,n'l'} - \lambda \delta_{nn'} \delta_{ll'}) \frac{\psi_{n'l'}}{(\xi_x - \tilde{\xi})}$$

(49)

where $\tilde{\xi} = \frac{E - \lambda}{\epsilon}$. The derivation of the dispersion relation from Eq. (49) appears to be physically more correct than from Eq. (11) because of the term $(\xi_x - \tilde{\xi})$ as discussed later. Eq. (49) is solved by substituting the series expansion of the collision operator in which the eigenvalues of terms of higher order than $\psi_{NL}$ are represented by the single eigenvalue $\lambda_{N+1,L+1}$. This procedure collapses the eigenvalue spectrum of all eigenvalues of higher order

$$(\epsilon I + \hat{K})a = 0$$

(50)

where the matrix elements of $\hat{K}$ correspond to

$$\hat{K}_{rs,sl} = \sum_{n' l'}^{N,L}(K_{rs,n'l'} - \lambda \delta_{rs} \delta_{sl}) \left( \psi_{nl}, \frac{\psi_{n'l'}}{\xi_x - \tilde{\xi}} \right)$$

$$= \sum_{n' l'}^{N,L} \beta_{rs,n'l'} \left( \psi_{nl}, \frac{\psi_{n'l'}}{\xi_x - \tilde{\xi}} \right)$$

(51)

where $\beta_{rs,n'l'} = K_{rs,n'l'} - \lambda \delta_{rs} \delta_{sl}$ and

$$R_{nl,n'l'} = \left( \psi_{nl}, \frac{\psi_{n'l'}}{\xi_x - \tilde{\xi}} \right)$$

$$= \pi^{-1/2} \int e^{-\xi_x^2} \psi_{nl} \psi_{n'l'} \frac{d\xi_x}{\xi_x - \tilde{\xi}}.$$  (52)

Eq. (51) is not an eigenvalue problem since the matrix $\hat{K}$ depends on $E$ and $\epsilon$. The integrals $R_{nl,n'l'}$ in Eq. (52) can be written in a closed form as a series involving the Plasma Dispersion function

$$Z(\tilde{\xi}) = \pi^{-1/2} \int \frac{e^{-\xi_x^2}}{\xi_x - \tilde{\xi}} d\xi_x$$

(53)

which can be computed numerically to high accuracy [41,42].

The ST method introduces two modifications to the WCU approach. The first is the use of the Gross–Jackson approximation of the collision operator in which the eigenvalues of terms of higher order than $\psi_{NL}$ are represented by the single eigenvalue $\lambda_{N+1,L+1}$. This procedure collapses the eigenvalue spectrum of all eigenvalues of higher order
than $\lambda_{NL}$ to the single value $\lambda_{N+1L+1}$. The second aspect, shared by the treatments of Foch and Ford [34], Buckner and Ferziger [4] and Skvortsov [43,44], involves the division by the drift term in Eq. (48) yielding Eq. (49). Sirovich and Thurber employed 3-, 5-, 8- and 11-moments in their model Boltzmann equation and reproduced the results of Euler, Navier–Stokes and Burnett approximations to hydrodynamics as well as a good agreement with experimental results in the rarefied region. The ST method also gives the same solutions as Grad’s 13-moment method in the hydrodynamic region but the two do not agree in the rarefied region [5]. A detailed comparison of the WCU and ST methods of the solution is presented in the next section.

2.8. Effects of ST modifications to the WCU method

The results obtained with the method proposed by Sirovich and Thurber are presented in Fig. 3. It demonstrates fairly good agreement with experiment at low orders (3 or 4 Burnett terms) and nonvanishing attenuation factors in the Knudsen region. The convergence of the ST solutions is markedly better than those of the WCU method (Fig. 1) which fails in the Knudsen region. Fig. 3A and B show that retaining only 12 terms in the ST method gives very good agreement with the experimental data.

The purpose of this work is to determine the validity of some assertions of Sirovich and Thurber regarding their method. It is instructive to illustrate the impact of the GJ treatment on the dispersion relation by examining some of the lower-order solutions. For a Maxwell gas, the 3-term approximation with the choice of Burnett functions $\psi_{00}, \psi_{01}$ and $\psi_{10}$ gives a collision operator of the following form

$$K^{(3)}[h] = -\lambda h + \frac{\lambda}{\pi^{3/2}} \int \left[a_{00} \times 1 + a_{01} \xi_1 \xi_x + a_{10} \frac{2}{3} \left(\xi^2 - \frac{3}{2}\right) \left(\xi_1^2 - \frac{3}{2}\right)\right] e^{-\xi_1^2} h(\xi_1) d\xi_1. \quad (54)$$

The $3 \times 3$ GJ matrix is

$$
\begin{pmatrix}
\epsilon + (\lambda_{00} - \lambda) R_{00,00} & (\lambda_{00} - \lambda) R_{00,01} & (\lambda_{00} - \lambda) R_{00,10} \\
(\lambda_{01} - \lambda) R_{10,00} & \epsilon + (\lambda_{01} - \lambda) R_{10,01} & (\lambda_{01} - \lambda) R_{10,10} \\
(\lambda_{10} - \lambda) R_{10,00} & (\lambda_{10} - \lambda) R_{10,01} & \epsilon + (\lambda_{10} - \lambda) R_{10,10}
\end{pmatrix}
\begin{pmatrix}
a_{00} \\
a_{01} \\
a_{10}
\end{pmatrix} = 0
\quad (55)
$$

where $R_{nl,n'l'}$ is given elsewhere [35]. The first few functions are

$$R_{00,00} = Z(\xi) \quad (56)$$
$$R_{01,00} = R_{00,01} = \sqrt{2} \left[1 + \xi Z(\xi)\right]$$
$$R_{01,01} = 2 \left[Z(\xi) + \xi \left[1 + \xi\right] Z(\xi)\right]$$
\[ R_{10,00} = R_{00,10} = \sqrt{\frac{2}{3}} \left[ \xi_0 + \left[ \frac{2}{3} \xi_0^2 - \frac{1}{2} \right] Z(\xi_0) \right] \]
\[ R_{10,01} = R_{01,10} = \sqrt{\frac{4}{3}} \xi_0 + \left[ \frac{4}{3} \xi_0^2 - \frac{1}{2} \right] Z(\xi_0) \]
\[ R_{10,10} = \left[ \frac{2}{3} \xi_0^4 - \frac{2}{3} \xi_0^2 + 2 \right] Z(\xi_0) + \xi_0^3 - \frac{1}{2} \xi_0. \]

If we set \( \lambda = \lambda_{22} \) as an approximation of the truncated part of the operator, we obtain a reasonable result for velocity and attenuation rates. In this case, \( \lambda_{00} = \lambda_{01} = \lambda_{11} = 0 \) and the dispersion relation can be computed from the roots of the secular determinant which is

\[ \epsilon^3 + \epsilon^2 \phi_3(\xi) + \epsilon \phi_2(\xi) + \phi_1(\xi) = 0 \]  \hspace{1cm} (57)

where

\[ \phi_1 = \frac{2}{3} \xi_0^3 + \frac{5}{3} \xi_0 + Z(\xi_0) \left( \frac{2}{3} \xi_0^4 + \frac{11}{6} \right) \]
\[ \phi_2 = -\frac{4}{3} \xi_0^2 - 2 - \frac{4}{3} \xi_0^3 + Z(\xi_0) \left( \frac{4}{3} \xi_0^2 + \frac{2}{3} \right) \]
\[ \phi_3 = \frac{2}{3} \xi_0^2 + Z(\xi_0) \left( \frac{2}{3} \xi_0^2 - \frac{5}{3} \right) - \frac{4}{3} Z(\xi_0)^2. \]

The complex roots of the complex function Eq. (57) were computed numerically using the Newton–Raphson method. The phase velocity and attenuation rate for 3-, 4-, 9- and 12-term GJ solutions are shown in Fig. 3A and B. The results agree well with experimental data [29] for forced sound in argon. In contrast to the WCU method which gives dispersion relations over the entire range of \( Kn \), the ST method fails to give solutions above a frequency referred to here as the cutoff frequency. For the 3-term solution, the cutoff is approximately \( Kn = 0.7 \). For higher-order approximations it is closer to \( Kn \sim 0.1 \) (Fig. 3A and B). A further discussion of high-frequency cutoffs is deferred to Section 2.9.

The ST method makes two modifications to the WCU method. The first modification uses the GJ approximation (Eq. (45)) that can be shown to affect only solutions obtained to low order. Sirovich and Thurber apply Eq. (45) to approximately preserve the truncated portion of the collision operator. The value of \( \lambda \) is unspecified, but Sirovich and Thurber base their argument on an approximate spectral representation, and consider \( \lambda \) to be the value for which all eigenvalues \( \lambda_{N+1L+1} \) and higher are approximated with a truncated spectrum.

The case of Maxwell molecules suggests another possible value for the choice of \( \lambda \). If one replaces \( \lambda \) with \(-\nu\), a dimensionless collision frequency, the RHS of Eq. (47) is the kernel of the Hilbert form of the Boltzmann equation,

\[ (E - \epsilon \xi_0 + \nu) h = \sum_{n,l,n',l'} a_{nl} (K^{nl}_{n'l'} - \nu \delta_{nn'} \delta_{ll'} + \nu \delta_{nn'} \delta_{ll'}) \psi_{n'l'} \]
\[ = \sum_{n,l,n',l'} a_{nl} K^{nl}_{n'l'} \psi_{n'l'} \]  \hspace{1cm} (59)

where

\[ K^{nl}_{n'l'} = K^{nl}_{nl'} + \nu \psi_{nl} \]
\[ = \pi^{-3/2} \int \int e^{-\xi_1^2} \left[ \psi_{nl}(\xi_1') + \psi_{nl}(\xi_1') - \psi_{nl}(\xi_1) \right] g \sigma d\Omega d\xi_1. \]  \hspace{1cm} (60)

Eq. (59) is, for the case of Maxwell molecules, identically the formulation of the sound dispersion problem suggested by Ford and Foch [34] and by Skvortsov [43,44]. It is useful to note that the 3-term approximation to the ST collision operator, Eq. (54), with \( \lambda = -\nu \) is identically the BGK model operator. Setting \( \lambda = 0 \) gives the WCU collision matrix on the RHS of Eq. (47). The ST method is, in effect, the division of the collision operator into two terms and moving one term over to the drift side prior to division of the RHS by the drift term.
Fig. 4. Graph of $\beta \omega^{-1} v_0$ versus $1/Kn$ for (A) 6-term approximation with $\lambda$ equal to $\lambda_{32}$ and $-\nu$, (B) 9-term approximation with $\lambda$ equal to $\lambda_{33}$, $-\nu$ and 0, and (C) 12-term approximation with $\lambda$ equal to $\lambda_{43}$, $-\nu$ and 0.

Figs. 4 and 5 show the effect the choice of $\lambda$ on the phase velocity and attenuation, respectively, for a set of ST solutions truncated at 6 ($N = 2$, $L = 1$), 9 ($N = 2$, $L = 2$) and 12 ($N = 3$, $L = 2$) terms. The corresponding values $\lambda = \lambda_{N+1L+1}$ in step Eq. (45) are $\lambda_{32} = -0.8949\nu$, $\lambda_{33} = -1.058\nu$ and $\lambda_{43} = -1.112\nu$.

There is some small variation in the phase velocity and attenuation depending on whether $\lambda$ is chosen as $\lambda_{N+1L+1}$ or $-\nu$ for 6- and 9-term approximations. No solutions were found with $\lambda = 0$ in the 6-term case (Figs. 4A and 5A). The 9-term solution shows some dependence on the choice of $\lambda$, especially in the Knudsen region. The choice of $\lambda = 0$ for the 9-term solution moves the cutoff from $Kn \approx 0.2$ to $Kn \approx 1$. The 12-term solution appears to be insensitive to the value $\lambda$ (Figs. 4C and 5C). This suggests that the influence of $\lambda$ on the solution declines as more terms are retained. The intended purpose of ST for introducing $\lambda$ in Eq. (45) is to increase the convergence of low-order solutions. As more terms are added, and the solutions converge, the inclusion of the term in $\lambda$ becomes unnecessary. This suggests that the choice of $\lambda$ is to a large degree arbitrary and that as more terms are used in the expansion and as the expansion converges, the use of the term $\lambda$ becomes redundant.

The second modification of Sirovich and Thurber is the division by the drift term in Eq. (49) and this appears to significantly affect the nature of the solution. Eq. (44) is of the form

$$L[h] = K[h]$$

where for forced sound, $(L = E - \epsilon(E)\xi_x)$ and $K$ is the Boltzmann collision operator. The problem is to determine the eigenvalues and eigenfunctions of Eq. (61) and ultimately, $\epsilon(E)$. Grad showed that the operator $\xi_x$ on the LHS has a continuous eigenvalue spectrum [45]. The operator $K$ on the RHS has a discrete eigenvalue spectrum for Maxwell molecules. In the present study, Eq. (44) is discretized by expressing $h$ in terms of a series expansion eigenfunctions of the RHS operator. This approach is convenient in that it gives easily-treated representations of the discretized operators, defined by the matrices $C$ and $K$ Eqs. (12) and (13). The discretization of $h$ in eigenfunctions of the RHS operator does not guarantee that the LHS operator, with a continuous spectrum, will or can be accurately represented in a discretized form. It appears that in the collisionless limit, the discrete representation is inadequate and the WCU method fails.
The reason the WCU method works in the hydrodynamic limit appears to be that the discrete spectrum of the collision operator dominates the solution for the collision-dominated hydrodynamic region.

Buckner and Ferziger [4] expanded $h$ in a complete set of eigenfunctions that represented both the discrete and continuous spectra of the linearized Boltzmann collision operator. They obtained reasonably good agreement with experiment for small and large Knudsen numbers in the range $10^{-2}$ to 100. However, their formalism gives poor agreement with experiment in the intermediate region $Kn \approx 1$ [46].

Solutions obtained with the WCU method in the Knudsen region appear to arise from a class of solutions that do not correspond to the physical system. The 483-moment solution of Pekeris [8] shows the attenuation $\alpha/\omega$ going as $1/\omega$ in the Knudsen region. This implies that for the WCU method, $\alpha$ is no longer a function of $\omega$ for large values of $\omega$, a fact that is inconsistent with the definition of a dispersion relation.

Sirovich and Thurber have modified the WCU method by first dividing Eq. (61) through out by $L$ and then discretizing the equation. This procedure gives a very different result than the WCU method. The difference can be noted by examining the forms of the respective matrix equations and the dispersion relations. The dispersion relation obtained from the 4-term ST method with $\lambda = 0$, analogous to the 4-term WCU is

$$
\epsilon - \lambda_{11} 2\sqrt{2} \left( Z \left( \frac{E}{\epsilon} \right) \left[ 4 \left( \frac{E}{\epsilon} \right)^5 + 6 \left( \frac{E}{\epsilon} \right)^4 + 2 \left( \frac{E}{\epsilon} \right)^2 + 16 \frac{E}{\epsilon} + 5 \right] + \left[ 4 \left( \frac{E}{\epsilon} \right)^3 + 6 \left( \frac{E}{\epsilon} \right)^2 + 2 \frac{E}{\epsilon} + \frac{137}{4} \right] \right) = 0.
$$

The difference is self-evident from a comparison between Eq. (21) obtained from the WCU method and Eq. (62) from the ST method as well as the phase velocity and attenuation factors that result from the respective solutions, as shown in Figs. 1 and 3. Division by the drift term prior to discretization appears to preserve the correct physical character of the solution.
2.9. High-frequency cutoff and free-molecule approximation

It can be demonstrated that under some conditions, there are no roots to the secular determinant for the ST matrix. If one considers a determinant of the ST matrix

\[ D(\bar{\xi}) = |eI - C(\bar{\xi})|. \]  

(63)

The existence of roots of the secular equation can be proven by obtaining the \textit{winding number} of the determinant for any given value of \( E \) (for the case of free sound, \( e \) would be the adjustable parameter). The winding theorem may be stated as follows: \textit{“The number of zeroes of a complex function \( D(\xi) \) of a complex variable \( \xi \) in a region of the complex \( \xi \)-plane for which \( D \) is an analytic function of \( \xi \) is equal to the number of times the representative point \( D \) circles the origin of the complex \( D \) plane as \( \xi \) is carried around a boundary region in the \( c \) plane”} [34]. If the winding theorem is applied above the so-called cutoff frequency, it can be shown that there are no plane wave solutions to the linearized Boltzmann equation for sound. The precise value of the cutoff frequency depends on the collision model and for the case of Maxwell molecules is around \( Kn \approx 10 \).

The winding theorem can be used to locate regions for which there are no roots of the secular determinant. The sound modes for forced sound waves lie in the range \( -1 \leq \beta v_0/\omega \leq 1 \) and \( 0 < \alpha v_0/\omega \leq 1 \). The domain of interest is the upper half of the complex \( \xi \)-plane. A large semicircle as shown in Fig. 6A bounds the solutions. A trajectory around a large semicircle requires computing \( D(\xi) \) for \(|\xi| \) large. Hand computation for low orders is feasible (Eq. (57)), since \( Z(\xi) \) has the asymptotic form

\[ Z(\xi) \sim -\sum_{n=0}^{\infty} \frac{\Gamma(n + \frac{1}{2})}{\Gamma(\frac{1}{2})} \xi^{-2n-1}. \]  

(64)

The \( D(\xi) \) trajectory resulting from a path \( \xi \) very close to and parallel with the real axis can also be computed by hand for low orders, since near the real axis, \( Z(\xi + i\phi) \) (\( \xi, \phi \) both real) has the asymptotic form

\[ \lim_{\phi \to 0^+} Z(\xi + i\phi) \sim -2e^{\xi^2} \int_{0}^{\xi} e^{x^2} dx + i\pi^{1/2} e^{-\xi^2}. \]  

(65)

Fig. 6B and C show winding plots for the 4-term approximation denoting the existence (Fig. 6B) of four roots below the cutoff frequency, corresponding to \( 1/Kn \approx 0.18 \) and none above it (Fig. 6C).

There is some evidence to suggest that the cutoff represents the high-frequency limit at which normal modes no longer physically exist. In collision-dominated systems, the impulse is carried as a plane wave by coherent collective modes. This is because particles have an opportunity to collide numerous times between oscillations. In collisionless or high-frequency situations, the impulse is carried by incoherent single-particle modes. There will, in the later case, be an insufficient number of collisions between oscillations to restore the system to equilibrium. Kahn and Mintzer recognized this problem and suggested that the reason for the breakdown is that the Maxwellian velocity distribution function constitutes a poor first approximation in the Knudsen region [3].

A simple model of a forced periodic disturbance in a collisionless system can be constructed as follows. The collisionless gas kinetic equation for a system with a disturbance in the \( x \)-direction is

\[ \frac{\partial f}{\partial t} + \xi x \frac{\partial f}{\partial x} = 0. \]  

(66)

Eq. (66) has a solution of the general form

\[ f = f^{(0)}[1 + h(t - x/\xi)]. \]  

(67)

The solution can be interpreted as a perturbed velocity distribution in which particles are emitted with the Maxwellian characteristic of the source but have a harmonic component along the axis of propagation (in this case the \( x \)-axis) \( h = Ae^{i\omega(t - x/\xi)} \) where \( A \) represents an amplitude of the perturbation. An impulse, \( P' \), generated by the disturbance is

\[ P'(x, t) = A\pi^{1/2} \int_{0}^{\infty} e^{i\omega(t - \xi/\xi)} e^{-\xi^2} d\xi. \]  

(68)

where the limits on the integral emphasize that only particles traveling in the +\( x \)-direction are considered. In Eq. (68), time and space dependencies are separable and
The impulse is assumed to decay through the random motion of the particles in the collisionless system. The magnitude of the impulse \( P' \) at \( x \) then depends on the magnitude of the impulse at the origin \( P'(0) \) and the distance \( x \) over which it has passed. A Beer–Lambert law for the decay of the impulse can be written

\[
P'(x) = P'(0) \exp \left( -\int_0^x k(x') \, dx' \right)
\]

where \( k \) is the propagation constant that describes the amplitude and phase of the impulse. Following the work of Meyer, \[29\], the term \( k \) is identically the wave number \( k = \beta + i \alpha \) where

\[
-k = \frac{\partial \ln[P'(x)/P'(0)]}{\partial x}
= \frac{\partial \ln[P'(x)]}{\partial x}
= \frac{\partial P'(x)}{P'(x)}
= \frac{\partial P'(x)}{ax}.
\]
When $P'(x)$ from Eq. (69) is substituted into Eq. (71), an expression for $k$ is obtained

$$k = -\int_0^\infty \frac{\partial}{\partial \xi} \left[ \cos \left( \frac{\omega \xi}{\xi_x} \right) + \sin \left( \frac{\omega \xi}{\xi_x} \right) \right] e^{-\xi^2} d\xi_x.$$  \hspace{1cm} (72)

The dimensionless propagation speed $\beta v_0/\omega$ and attenuation rate $\alpha v_0/\omega$ are obtained from the real and imaginary parts of Eq. (72) which, following some manipulation are found to be

$$\frac{\beta v_0}{\omega} = -\frac{I(\cos \frac{\omega \xi}{\xi_x}) I'(\cos \frac{\omega \xi}{\xi_x}) + I(\sin \frac{\omega \xi}{\xi_x}) I'(\sin \frac{\omega \xi}{\xi_x}) \sqrt{2}}{I(\cos \frac{\omega \xi}{\xi_x})^2 + I(\sin \frac{\omega \xi}{\xi_x})^2 \sqrt{2}},$$

$$\frac{\alpha v_0}{\omega} = -\frac{I'(\cos \frac{\omega \xi}{\xi_x}) I(\sin \frac{\omega \xi}{\xi_x}) - I'(\sin \frac{\omega \xi}{\xi_x}) I(\sin \frac{\omega \xi}{\xi_x}) \sqrt{2}}{I(\cos \frac{\omega \xi}{\xi_x})^2 + I(\sin \frac{\omega \xi}{\xi_x})^2 \sqrt{2}}.$$  \hspace{1cm} (73)

where

$$I(g(\xi_x, \omega, x)) = \int_0^\infty g(\xi_x, \omega, x) e^{-\xi^2} d\xi_x.$$  \hspace{1cm} (74)

and $I' = \frac{1}{\omega} \frac{\partial I}{\partial \omega}$. Meyer and Sessler computed $\beta/\omega$ and $\alpha/\omega$ numerically for the case of $\omega\xi$ large [29] and obtained

$$\frac{\beta v_0}{\omega} \approx 0.45 \quad \text{and} \quad \frac{\alpha v_0}{\omega} \approx 0.22.$$  \hspace{1cm} (75)

which was in excellent agreement with their experimental result.

Fig. 3 shows that the asymptotic values for phase velocity and attenuation, Eq. (75) correspond closely to the converged values obtained for the collision-dominated system at the cutoff point. The fact that phase velocities and attenuation rates near the cutoff agree with the free-molecule result suggests that the observed cutoff may represent the limit of the collisionless region.

3. Summary

A detailed comparison of the available methods of solution of the Boltzmann equation for the description of the propagation of sound waves in a monatomic gas has been carried out. We have demonstrated and explained the rapid convergence of solutions obtained with the formalism proposed by Sirovich and Thurber [5–8] in comparison with the calculations by Wang Chang and Uhlenbeck [30,34] which converge very slowly as shown by Perkeris [31,32]. The method proposed by Alexeev [13,14] is not useful. We have compared with the available experimental data and we obtain reasonable agreement with the Maxwell molecule inverse fourth power potential. The failure of the ST method to yield solutions for high sound frequencies is shown to be consistent with experimental data for sound waves around the collisionless limit. It is clear that there is an urgent need for additional experimental data for more detailed comparisons with theoretical models.

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