

Continuum description of rarefied gas dynamics. II. The propagation of ultrasound

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The equations of fluid dynamics developed in Paper I [X. Chen, H. Rao, and E. A. Spiegel, *Phys. Rev. E* **64**, 046308 (2001)] are applied to the study of the propagation of ultrasound waves. There is good agreement between the predicted propagation speed and experimental results for a wide range of Knudsen numbers.

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I. STATEMENT OF THE EQUATIONS

Modern theoretical studies of the influence of dissipation on the propagation of sound on the basis of the Navier-Stokes equations may be said to have begun with the work of Kirchhoff [1]. A principal aim of that and subsequent studies is to determine how the propagation speed and the rate of dissipation of the waves depend on their frequencies. For this problem, the predictions from the standard Navier-Stokes (NS) equations of fluid dynamics do not agree well with experiments when the periods of the sound waves become as short as the mean flight times of the particles of the gas, that is, when we enter the ultrasound regime.

There are two directions from which to enter that regime. We can begin with a gas of freely steaming particles and introduce weak interactions among them. In that case, we may with Uhlenbeck and Ford [2] ask, ‘‘How is it possible to impose on the random motion of the molecules the ordered motion . . . which a sound wave represents?’’ In the modern language of dynamical systems theory, this could be seen as a problem of synchronization in which we witness increasing numbers of particles going into cooperative motion until all are engulfed. On the other hand, we may start from the case of continuum mechanics and attempt to extend the validity of that description to the case of longer and longer mean free paths. It is unlikely that in either case we can successfully traverse the full range of possible conditions, but we may expect to encounter an interesting transition between the two regimes.

In this paper, we examine how well the fluid dynamical description of Paper I of this series [3] extends into the domain where the particle mean free paths are comparable to the characteristic macroscopic length scale of the medium. In Paper I, we derived an extension of the fluid dynamical equations that we hope may offer an improvement of this kind and, in the present paper, we study their linear form and the resultant dispersion relation for sound waves. In this section, we restate the equations given in Paper I before going on to the straightforward determination of the dispersion relation they imply for the linear theory of sound waves.

The basic form of the macroscopic equations derived

from kinetic theory, are [4–6]

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (1.1)$$

$$\rho(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) + \nabla \cdot \mathbf{P} = \mathbf{0}, \quad (1.2)$$

$$\frac{3}{2} \rho R(\partial_t T + \mathbf{u} \cdot \nabla T) + \mathbf{P} : \nabla \mathbf{u} + \nabla \cdot \mathbf{Q} = 0, \quad (1.3)$$

where ρ is mass density, \mathbf{u} is the velocity field, T is the temperature, \mathbf{P} is the pressure tensor, \mathbf{Q} is the heat flux vector, and the colon stands for a double dot product. We have not included an external force.

These equations express Newton’s laws of motion for a continuum in phenomenological theories and they are a formal consequence of most kinetic theories. Where approaches to the derivation of these equations from kinetic theory may differ is in the expressions for the higher moments, \mathbf{P} and \mathbf{Q} . The derivations from kinetic theory are important since they provide formulas for the transport coefficients that appear in the specific expressions for the pressure tensor and the heat flux. However, not all treatments of the kinetic theory give the same explicit formulas for \mathbf{P} and \mathbf{Q} , there being differences of degree and style of the approximations used. Of course, when the mean free path of the constituent particles is sufficiently short compared to all macroscopic lengths in the problem, there is no real disagreement, since the standard Navier-Stokes forms work well enough for most purposes. But when the macroscopic lengths become short and are comparable to the mean free paths of the particles, those standard results do not agree with experiment, as we shall see. Therefore we must ask whether there is a continuum approximation that may provide improved treatments of such problems.

To test whether the expressions for \mathbf{P} and \mathbf{Q} derived in Paper I from the relaxation model of kinetic theory [7,8] may fulfill this need, we here apply them to study of the propagation of ultrasound. In the relaxation model, the relaxation time τ may be taken to be of the order of the mean flight time of particles, where the mean speed is of the order of the speed of sound. Then, we have

$$\tau = \frac{\alpha}{\rho\sqrt{T}}, \quad (1.4)$$

where α is a constant that depends on the collision cross section and the gas constant and we have ignored a possible dependence of the particle cross-section time on particle speed.

The results in Paper I are based on an expansion in τ , up to first order. Those expansions led to a pressure tensor,

$$\mathbf{P} = \left[p - \mu \left(\frac{D \ln T}{Dt} + \frac{2}{3} \nabla \cdot \mathbf{u} \right) \right] \mathbf{I} - \mu \mathbf{E}, \quad (1.5)$$

where

$$p = R\rho T, \quad (1.6)$$

R is the gas constant,

$$E^{ij} = \frac{\partial u^i}{\partial x_j} + \frac{\partial u^j}{\partial x_i} - \frac{2}{3} \nabla \cdot \mathbf{u} \delta^{ij}, \quad (1.7)$$

$$\mu = \tau p \quad (1.8)$$

is the viscosity, and $D/Dt = \partial_t + \mathbf{u} \cdot \nabla$. The result for μ , together with Eq. (1.4), implies Maxwell's conclusion that viscosity does not depend on density for simple gases. For the heat flux, we obtained

$$\mathbf{Q} = -\eta \nabla T - \eta T \nabla \ln p - \frac{5}{2} \mu \frac{D\mathbf{u}}{Dt}, \quad (1.9)$$

where $\eta = \frac{5}{2} \mu R$ is the conductivity. Both Eq. (1.5) and Eq. (1.9) carry errors of order τ^2 that are not indicated explicitly.

These formulas for \mathbf{P} and \mathbf{Q} are not expressed explicitly in terms of the fluid fields. Rather, their expressions involve some of the same time derivatives of these fields that appear in the fluid equations. Here is the central difference between our results and those obtained in the Chapman-Enskog approach. In the latter, partial derivatives with respect to time are eliminated by the use of lower order results. Though we do not use that elimination procedure in deriving the closure relations, we can nevertheless readily recover the Navier-Stokes results from ours, when $\tau \rightarrow 0$, as we described in paper I. However, even though both theories formally have first-order accuracy in τ , the results from them are significantly different at Knudsen numbers of order unity, as we shall see in what follows.

II. THE LINEAR THEORY

We consider the evolution of perturbations on a uniform medium and define perturbation variables ϕ , θ , and ϖ through the relations

$$\rho = \rho_0(1 + \phi), \quad T = T_0(1 + \theta), \quad \text{and} \quad p = p_0(1 + \varpi), \quad (2.1)$$

where ρ_0 , T_0 , and p_0 are the constant background values of the thermodynamic fields. The perturbation quantities all

have small amplitudes with, for example, $|\phi| \ll 1$. From the linearization of Eq. (1.6) we obtain

$$\varpi = \phi + \theta. \quad (2.2)$$

We further assume that there is no background motion so that \mathbf{u} is small and needs no subscripts.

In analogy with Eq. (2.1) we write for the pressure tensor, the linearized form

$$\mathbf{P} = p_0 \mathbf{I} + \mathbf{T}, \quad (2.3)$$

where

$$\mathbf{T} = \varpi \mathbf{I} - \tau (\partial_t \theta + \frac{2}{3} \nabla \cdot \mathbf{u}) \mathbf{I} - \tau \mathbf{E}, \quad (2.4)$$

where τ is evaluated for the state variables of the background medium and \mathbf{E} is small. Similarly, since there is no zeroth order heat flux, we get for the linearized heat flux,

$$\mathbf{Q} = -\eta_0 T_0 \nabla (\theta + \varpi) - \frac{5}{2} \mu_0 \partial_t \mathbf{u}. \quad (2.5)$$

The quantities $\mu_0 = \tau p_0$ and η_0 are the viscosity and conductivity evaluated in terms of the state variables for the constant background medium.

The linearization of Eq. (1.1) is

$$\partial_t \phi + \nabla \cdot \mathbf{u} = 0. \quad (2.6)$$

A compact form of the linearized Eq. (1.2) is

$$\rho_0 \partial_t \mathbf{u} + p_0 \nabla \cdot \mathbf{T} = \mathbf{0}. \quad (2.7)$$

When we take the divergence of Eq. (2.7) and use Eq. (2.6), find that

$$\rho_0 \partial_t^2 \phi - p_0 \nabla \nabla : \mathbf{T} = 0. \quad (2.8)$$

From Eq. (2.4) we find that

$$\nabla \cdot \mathbf{T} = \nabla \varpi - \tau \partial_t \nabla \theta - \frac{2}{3} \tau \nabla \cdot (\nabla \cdot \mathbf{u}) - \tau \nabla \cdot \mathbf{E}. \quad (2.9)$$

We see from Eq. (1.7) that

$$\nabla \cdot \mathbf{E} = \nabla^2 \mathbf{u} + \frac{1}{3} \nabla \cdot (\nabla \cdot \mathbf{u}). \quad (2.10)$$

Then, with the help of Eq. (2.6), we find

$$\nabla \cdot \mathbf{T} = \nabla \varpi - \tau \partial_t \nabla (\theta - \phi) - \tau \nabla^2 \mathbf{u}. \quad (2.11)$$

On using Eq. (2.6) again, we find that

$$\nabla \nabla : \mathbf{T} = \nabla^2 \varpi - \tau \partial_t \nabla^2 (\theta - 2\phi), \quad (2.12)$$

which we may introduce into Eq. (2.8). Next we define the Laplacian speed of sound a and the kinematic viscosity ν_0 as in

$$a^2 = \frac{p_0}{\rho_0} \quad \text{and} \quad \nu_0 = \frac{\mu_0}{\rho_0}. \quad (2.13)$$

We then obtain the dissipative wave equation

$$(\partial_t^2 - a^2 \nabla^2 - 2\nu_0 \partial_t \nabla^2) \phi + (\nu_0 \partial_t - a^2) \nabla^2 \theta = 0. \quad (2.14)$$

To complete this discussion, it is useful to introduce the thermal diffusivity

$$\kappa_0 = \frac{\eta_0}{\rho_0 C_p}, \quad (2.15)$$

where $C_p = \frac{5}{2}R$. Thus, $\eta_0 T_0 = \frac{5}{2} p_0 \kappa_0$. This is used in the linearized heat equation,

$$\frac{3}{2} p_0 \partial_t \theta + p_0 \nabla \cdot \mathbf{u} + \nabla \cdot \mathbf{Q} = 0, \quad (2.16)$$

where we may write

$$\nabla \cdot \mathbf{Q} = -\frac{5}{2} p_0 \kappa_0 \nabla^2 (\phi + 2\theta) + \frac{5}{2} \rho_0 \nu_0 \partial_t^2 \phi. \quad (2.17)$$

Since $\nu_0 = a^2 \tau$, we then find

$$\left(\tau \partial_t - \frac{10}{3} \frac{a^2 \tau^2}{\sigma} \nabla^2 \right) \theta + \left(\frac{5}{3} \tau^2 \partial_t^2 - \frac{2}{3} \tau \partial_t - \frac{5}{3} \frac{a^2 \tau^2}{\sigma} \nabla^2 \right) \phi = 0, \quad (2.18)$$

where

$$\sigma = \frac{\nu_0}{\kappa_0} \quad (2.19)$$

is the Prandtl number of the undisturbed medium.

Finally, to further simplify the appearance of these formulas, we let the unit of time be τ and the unit of length be $a\tau$. Then our linearized equations for sound waves are

$$(\partial_t^2 - \nabla^2 - 2\partial_t \nabla^2) \phi + (\partial_t - 1) \nabla^2 \theta = 0, \quad (2.20)$$

$$\left(5\partial_t^2 - \frac{5}{\sigma} \nabla^2 - 2\partial_t \right) \phi + \left(3\partial_t - \frac{10}{\sigma} \nabla^2 \right) \theta = 0. \quad (2.21)$$

For comparison we note that the analogous linear equations for the Navier-Stokes case (with zero bulk viscosity) are

$$(\partial_t^2 - \nabla^2 - \frac{4}{3} \partial_t \nabla^2) \phi - \nabla^2 \theta = 0, \quad (2.22)$$

$$-2\partial_t \phi + \left(3\partial_t - \frac{5}{\sigma} \nabla^2 \right) \theta = 0. \quad (2.23)$$

III. THE DISPERSION RELATIONS

We may seek solutions to the linear equations (2.20) and (2.21) in which ϕ and θ vary like $\exp(ikx - st)$. Since the mean free path is the unit of length, the wave number k , which is nondimensional, is effectively the Knudsen number for this problem. The dispersion relation is

$$(3 + 5k^2)s^3 - \left(\frac{10}{\sigma} - 1 \right) k^2 s^2 + 5 \left(\frac{5}{\sigma} k^2 + 1 \right) k^2 s - \frac{5}{\sigma} k^4 = 0. \quad (3.1)$$

For comparison, we report that the dispersion relation for the Navier-Stokes equations is

$$3s^3 - \left(\frac{5}{\sigma} + 4 \right) k^2 s^2 + 5 \left(\frac{4}{3\sigma} k^2 + 1 \right) k^2 s - \frac{5}{\sigma} k^4 = 0. \quad (3.2)$$

A. Frequencies

To get a feel of what these results mean, we look at free modes for which k is real. Then we set $s = i\omega + \alpha$ where α and ω are also real. When we introduce this into Eq. (3.1) we find that there is a (thermal) mode with $\omega = 0$ and a pair of (acoustic) modes whose frequencies satisfy

$$\omega^2 = 3\alpha^2 - \frac{2(10 - \sigma)}{\sigma(3 + 5k^2)} k^2 \alpha + \frac{5(\sigma + 5k^2)}{\sigma(3 + 5k^2)} k^2, \quad (3.3)$$

which gives the frequencies of sound waves. As we may confirm, α is of order unity for large k and it grows in proportion to k^2 for small k . Hence, for both very large and very small k , the last term on the right of Eq. (3.3) is the largest one on that side. So we may write the uniform approximation

$$\omega^2 = \frac{5(\sigma + 5k^2)}{\sigma(3 + 5k^2)} k^2. \quad (3.4)$$

For small k , this gives the phase speed $\omega/k = \pm \sqrt{5/3}$, which is the usual speed of sound for an adiabatic sound wave, as is to be expected for very long wavelengths. For large k , we obtain the phase speed $\omega/k = \pm \sqrt{5/\sigma}$.

For the NS equations with zero bulk viscosity there is the same number of modes: a thermal mode with zero frequency and sound waves with

$$\omega^2 = 3\alpha^2 - \frac{2}{3} \left(\frac{5}{\sigma} + 4 \right) k^2 \alpha + \frac{5}{3} \left(\frac{4k^2}{3\sigma} + 1 \right) k^2. \quad (3.5)$$

As expected, the two sets of equations agree in the limit of very small k , where the NS equations return the phase speed $\pm \sqrt{5/3}$. But for large k , the differences between the two theories become qualitative. With the Navier-Stokes equations, we find that at large k , instead of reaching a finite limit, the phase speed is proportional to k for large k . As we shall see when we look at the experimental results, the NS prediction is qualitatively wrong; the phase speed goes to a finite value at large k .

B. Damping rates

The equation for the damping rate is

$$(3 + 5k^2)\alpha^3 - \left(\frac{10}{\sigma} - 1 \right) k^2 \alpha^2 - \left[3(3 + 5k^2)\omega^2 - 5 \left(1 + \frac{5}{\sigma} k^2 \right) k^2 \right] \alpha + \left(\frac{10}{\sigma} - 1 \right) k^2 \omega^2 - \frac{5}{\sigma} k^4 = 0. \quad (3.6)$$

For the thermal mode, for which $\omega = 0$, we find the damping rates $\alpha = k^2/\sigma$ for small k and $\alpha = 1/5$ for large k . Thus,

there is very little damping for long waves while short waves are damped on the collisional time scale. Moreover, on examination of these two limits, we see that they both emerge from the balance of the same two terms in Eq. (3.6). Hence we may write the approximate formula

$$\alpha = \frac{k^2}{\sigma + 5k^2} \quad (3.7)$$

as a reasonable approximation to the damping rate for all k , in the thermal mode.

Similarly, in the case of sound waves, we see that α is also the result of the balance between the same two terms in Eq. (3.6) in the limits of large and small k . Hence, we find that for sound waves, to good approximation, the damping rate is given by

$$\alpha = \frac{(10 - \sigma)k^2\omega^2 - 5k^4}{3\sigma(3 + 5k^2)\omega^2 - 5k^2(\sigma + 5k^2)}, \quad (3.8)$$

where ω is given in Eq. (3.4). For long wavelengths, the damping is again slight since it goes to zero like $[(7 - \sigma)/(6\sigma)]k^2$. For large k , we obtain the finite limit $\alpha = (5 - \sigma)/(5\sigma)$.

For the Navier-Stokes equations, the damping rate is given by

$$3\alpha^3 - \left(\frac{5}{\sigma} + 4\right)k^2\alpha^2 + \left[5\left(\frac{4k^2}{3\sigma} + 1\right)k^2 - 9\omega^2\right]\alpha + \left(\frac{5}{\sigma} + 4\right)k^2\omega^2 - \frac{5}{\sigma}k^4 = 0. \quad (3.9)$$

The damping rate for the acoustic modes also goes like k^2 for small k for both the thermal mode and the acoustic modes. For the acoustic modes, the damping rate is $\alpha = [(2\sigma + 1)/(3\sigma)]k^2$, so that we get the same wave number dependence, but with a different coefficient than is obtained from our equations in the small k limit. However, for increasing k , the NS damping rates *grow* like k^2 for sound waves, which is in disagreement with experiment [9].

IV. COMPARISON WITH EXPERIMENT

Though the study of free modes in the previous section is intuitively clear, it does not directly represent the way experiments on sound propagation are usually carried out. In the experiments, it is more typical that one drives the fluid at a real, fixed frequency and then studies the propagation of waves in space. The forcing may be accomplished by vibrating the end wall of a tube containing gas at a fixed (real) frequency ω and observing the propagation down the tube. To model this procedure in full detail would involve a careful treatment of the forcing procedure, which usually requires attention to boundary conditions. However, in this first reconnaissance of the way our equations describe sound waves, we shall adopt a standard theoretical practice [1] and simply fix the wave frequency ω in the dispersion relation and compute the resulting k , which will typically be com-

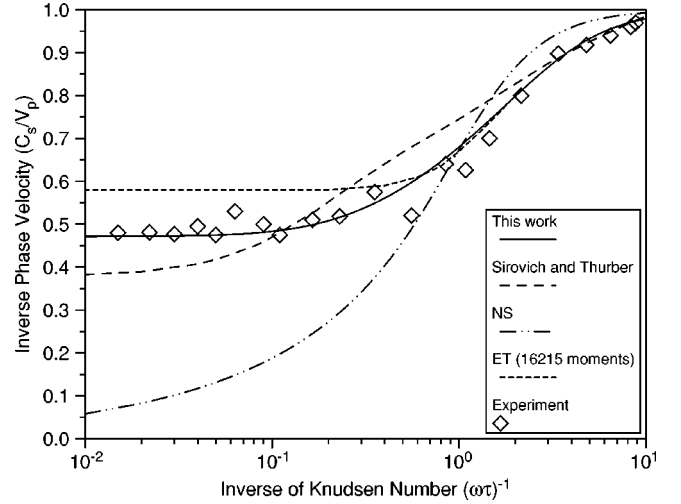


FIG. 1. The inverse phase velocity as a function of inverse frequency.

plex. Thus, in Eq. (3.1) we let $s = i\omega$ and we find that the equation for k becomes

$$\frac{5}{\sigma}(1 - 5i\omega)k^4 + \left[5i\omega^3 - 5i\omega - \left(\frac{10}{\sigma} - 1\right)\omega^2\right]k^2 + 3i\omega^3 = 0. \quad (4.1)$$

We may similarly obtain such an equation for the NS case, Eq. (3.2). In order to emphasize the results for large Knudsen number we plot the results in the manner used, for example, by Cercignani [4]. That is, we introduce the quantity

$$K^2 = \frac{5k^2}{3\omega^2}, \quad (4.2)$$

where K is a normalized inverse propagation speed. The factor $5/3$ is included so that the phase speed is nondimensionalized on the Laplacian (or adiabatic) speed of sound, rather than the Newtonian (or isothermal) speed of sound as above. Then we find that

$$(1 - 5i\omega)K^4 + \frac{\sigma}{3}\left[5i\left(\omega - \frac{1}{\omega}\right) - \left(\frac{10}{\sigma} - 1\right)\right]K^2 + \frac{5\sigma i}{3\omega} = 0. \quad (4.3)$$

To see how this representation contains the results for free modes, we note that, in the limit $\omega \rightarrow 0$, Eq. (4.3) reduces to $K^2 = 1$. That is, for low frequencies, the usual adiabatic sound speed is recovered. In the (more interesting) opposite limit, $\omega \rightarrow \infty$, we obtain $K^2 = \sigma/3$ for the propagative modes. Thus we see that, in the limit of forcing at high frequency, sound waves propagate with phase speeds $\pm \sqrt{\sigma/3}$, independently of frequency. The data shown in the accompanying figure (Fig. 1) confirm this independence of frequency (or wave number) of the speed of propagation of ultrasound. The observed nondimensional phase speed is 0.47.

The Prandtl number found from the relaxation model of kinetic theory, either by the methods of Chapman and Enskog or those described in paper I, is unity. With this value, we obtain 0.51 for the limiting phase speed, so this repre-

sents a small quantitative error. However, the value of σ found in kinetic theory depends on the atomic model used, that is, on the nature of the collision term. Though the relaxation model gives the explicit value unity for σ , the value found with the traditional Boltzmann equation for hard spheres is $2/3$. This difference has nothing to do with the approximation method (our procedure gives $\sigma=2/3$ when applied to the Boltzmann equation) but is a consequence of the nature of the form of the atomic interactions that is adopted. We therefore follow a common practice of putting the empirical Prandtl number into the theoretical results when comparing with experiments. Since the experimental data we shall refer to are for noble gases whose values of σ are 0.6 or 0.7 we shall here adopt the value $\sigma=2/3$ suggested by the Boltzmann equation. When we use that value of the Prandtl number in evaluating the phase speed, we obtain $K = \sqrt{2}/3 = 0.471$. Even without this adjustment, the results for the propagation of ultrasound are good, but we would propose to anyone thinking of using our equations from this first-order development from the relaxation equation to introduce this phenomenological improvement of the theory.

In the accompanying figure (Fig. 1), we show the variation of $\text{Re } K$ as a function of $1/\omega$ from a number of sources. The experimental values [10,11] are indicated as individual points (the diamonds) and they appear to be tending toward a nonzero constant value at high frequency. This is qualitatively in accord with our results, here shown as a solid line for the case of $\sigma=2/3$, and it is in stark disagreement with the prediction from the Navier-Stokes equations (long dashes with double dots), which predict that $\text{Re } K$ goes to zero like

$1/\omega$. Since our limiting value for $\text{Re } K$ was found to be $\sqrt{\sigma/3}$, the remarkable agreement of our results with experiment owes something to our using the experimental value of $2/3$ for σ for limiting value $\text{Re } K \rightarrow 0.47$. Nevertheless, even without this choice, the results would be adequate and comparable to those shown for the moment method [12] with 16 215 moments (short dashes). Other theoretical studies of ultrasound are based on direct solution of the Boltzmann equation [4,2] and we show the results of Sirovich and Thurber [13] obtained in this way (medium dashes), for which the Prandtl number automatically has the value $2/3$.

V. CONCLUSION

In the study of the thermal damping of sound waves by electromagnetic radiation [14], one finds that, for thermal times much less than the acoustic period, sound propagates at the isothermal speed of sound with negligible dissipation. In the opposite limit of long thermal times, there is also little dissipation, but propagation is at the adiabatic speed of sound. The experiments, and the solution of the Boltzmann equation show similar behavior when the relevant parameter is the ratio of the collisional relaxation time to the acoustic period. Our equations, as well as those of the moment method (with tens of thousands of moments), reproduce this behavior but the Navier-Stokes equations do not. Moreover, when the Prandtl number is chosen to be that of the experimental gas, the quantitative agreement becomes very good. In the next installment of this series, we shall compute the profile of a stationary shock wave. As we shall see, the agreement with the experiments is good in that case too.

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