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DHARMAPALA, APARNA. Numerical Analysis of the Kinetic Theory of Sound Propagation in a Simple Monatomic Gas (1975)  
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The main purpose of this research is to develop the numerical techniques for calculating the absorption and dispersion of sound propagation in a simple monatomic gas. We approach the problem by using the Linearized B.G.K. model proposed by Bhatnagar, Gross, and Krook. To avoid mathematical complexity we consider only three terms in the model equation. After lengthy mathematical formulation we obtain a set of linear equations in the general eigenvalue-eigenvector form. Solution of this yields the absorption and dispersion in terms of the rarefaction parameter. Numerical methods are discussed for solving the eigenvalue equation and for developing a PL/1 computer program for calculating the absorption and dispersion of sound. We discuss some possible difficulties which may be encountered in numerical analysis.

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APPROVAL PAGE

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CHAPTER I  
INTRODUCTION

The kinetic theory of plane sound wave propagation in simple monatomic gaseous mixture has received increasing attention in recent years. Our research is a study of the numerical methods for calculating the absorption and dispersion of a sound wave propagating in a simple monatomic gas. The experimental procedure for measuring the absorption and dispersion of the sound wave through a gas is discussed below.

A cylindrical tube containing the gas is fitted at one end with a small, fixed speaker and with a microphone probe which can be moved along the axis of the tube. An oscillator provides the energy for the speaker, and an oscilloscope is used to display the disturbance detected by the microphone. A scale along the tube and a pointer on the microphone probe serve to indicate the position of the microphone. Absorbent material in the end of the tube opposite the speaker is used to minimize reflection. The speed,  $c$ , of sound propagation is obtained by measuring the frequency,  $\omega$ , of the oscillator and the wave length,  $\lambda$ , of the wave. The latter can be obtained by measuring the distance between the microphone positions which give in-phase and out-of-phase

Lissajous's figures. The absorption coefficient,  $\alpha$ , is obtained by measuring the attenuation rate per unit length.

Physically the dispersion refers to the degree to which the speed of the wave deviates from the adiabatic value,  $c_0$  (low frequency sound speed), and the absorption refers to the amount by which the amplitude of the wave is changed. The dispersion and absorption are commonly written as dimensionless quantities and expressed as  $c_0/c$ , and  $\alpha c_0/\omega$  respectively. Therefore, once  $c$ ,  $\omega$ ,  $\alpha$ , and  $c_0$  are measured the dispersion and absorption of sound can easily be obtained. Here, we introduce a new independent variable,  $\kappa = p/\mu\omega = \nu/\omega$ , called the rarefaction parameter, where  $p$  is the pressure inside the tube,  $\mu$  is the coefficient of viscosity (which is a constant), and  $\nu$  is the collision frequency. The pressure inside the tube is varied in order to get the dispersion and absorption at different values of  $\kappa$ .

The kinetic theory of plane sound wave propagation has been described by the classical theory of Stokes and Kirchhoff.<sup>1</sup> Sound propagation by its very nature is a molecular<sup>2</sup> effect. But until the work of Wang Chang and Uhlenbeck<sup>2</sup> all attempts were essentially hydrodynamic. Wang Chang and Uhlenbeck worked with Boltzmann's equation but applied some approximations (such as a low sound frequency in comparison with the collision frequency) which are valid only for the macroscopic region. Thus, their work was also limited to the hydrodynamical region.

From the results of Sirovich's<sup>3</sup> report it is clear that a complete dispersion theory of sound propagation using the Boltzmann equation is unfeasible. The reason is that solutions to the Boltzmann equation are very hard to obtain without making some approximations which are only valid for macroscopic cases. In other words, these approximations are good for the low frequency region only. For the higher frequency region the solutions are not valid. It is our goal to obtain a description valid throughout the entire frequency range.

To accomplish this the Boltzmann's equation is discarded in favour of certain kinetic models suggested by Gross and Jackson<sup>4</sup>. These model equations are capable of reproducing the Euler, Navier-Stokes, Burnett and thirteen moment equations.<sup>3</sup> These moment equations can yield solutions without any approximation in the hydrodynamical region. The more terms that are taken in the model equation, the more accurately it describes the physical situation. The complete collision integral describes the physical situation accurately, whereas the model equation approximates it.

By solving the model equation we can obtain the dispersion relation in eigenvalue-eigenvector form. The solution of the dispersion relation yields the physical properties of the propagating sound wave. The order of the matrix in the eigenvalue equation increases as the number of terms in model equation increases.

We approach the problem by using the Linearized B.G.K.<sup>5</sup> model proposed by Bhatnagar, Gross, and Krook. To avoid mathematical complexity we considered only three terms (for the particle density, the flow velocity and the temperature) in the model equation. Thus, we make the numerical calculations much simpler. Once the computer program is developed for this simple case, then the number of terms in the model equation can be increased to obtain better results from the same computer program.

In Chapter II starting with the Linearized Krook model we develop an eigenvalue equation, which in turn gives us the dispersion relation. In Chapter III we discuss the numerical methods for solving the eigenvalue equation and calculating the absorption and dispersion of sound with the obtained solution. Finally, in Chapter IV we present conclusions and a brief summary of the entire research.

## CHAPTER II

## MATHEMATICAL FORMULATIONS

## A. The Krook Model

We begin with the Boltzmann equation for a gas of Maxwell molecules. In this model the collision term in the Boltzmann equation is approximated by a much simpler expression which predicts behaviour a lot like full collision integral. The approximation is

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = \left( \frac{\partial f}{\partial t} \right)_c = \nu (f_m - f), \quad (1)$$

where  $\nu$  is the collision frequency of the gas, assumed to be a constant;  $f$  is the distribution function; and  $f_m$  is the Maxwellian distribution function. Both  $f$  and  $f_m$  are functions of  $\vec{r}$ ,  $\vec{v}$ , and  $t$ . The Maxwellian distribution function can be expressed as

$$f_m(\vec{r}, \vec{v}, t) = n \left( \frac{\lambda}{\pi} \right)^{3/2} e^{-\lambda v^2}, \quad (2)$$

where  $n(\vec{r}, t)$  is the particle density of the gas, and is defined by

$$n(\vec{r}, t) = \int f(\vec{r}, \vec{v}, t) d\vec{v}; \quad (3)$$

and where the peculiar velocity,  $\vec{s}$ , is given by

$$\vec{s} = \vec{v} - \vec{u}(\vec{r}, t), \quad (4)$$

where the average velocity,  $\vec{u}$ , is defined by

$$\vec{u}(\vec{r}, t) = \langle \vec{v} \rangle = \frac{1}{n} \int \vec{v} f(\vec{r}, \vec{v}, t) d\vec{v} . \quad (5)$$

Also, in Eq. (2),  $\lambda$  is given by

$$\lambda = \frac{m}{2kT} ,$$

where  $k$  is the Boltzmann's constant, and  $T(\vec{r}, t)$  is the temperature of the gas and is defined by

$$\frac{3}{2} kT(\vec{r}, t) = \frac{1}{n} \int \frac{1}{2} m v^2 f(\vec{r}, \vec{v}, t) d\vec{v} . \quad (6)$$

If Eq. (1) were used to develop a system of moment equation, the hydrodynamic, or conservation equations, i.e., the equations for  $n$ ,  $\vec{u}$ , and  $T$ , the results would be the same as obtained using the exact expression for collision integral. The left hand side of the moment equations would obviously be the same since the relaxation time approximation does not change the left hand side of the Boltzmann equation.

Now let us consider a new arbitrary function,  $Q$ , which is a function of  $\vec{r}$ ,  $\vec{v}$ , and  $t$ , and let  $\Delta Q$  be the average rate of change of  $Q$  per unit volume due to collisions. Then  $\Delta Q$  is given by

$$\Delta Q = \int Q \left( \frac{\partial f}{\partial t} \right)_c d\vec{v} .$$

Therefore, for the Krook model we can write

$$\Delta Q = \nu \int Q (f_m - f) d\vec{v} . \quad (6.5)$$

By setting  $Q$  equal to  $1$ ,  $m\mathcal{A}_i$ , and  $\frac{1}{2}m\mathcal{A}^2$  respectively into Eq. (6.5) we arrive at the following relations:

$$\begin{aligned}\Delta(1) &= \nu \int (f_m - f) d\vec{v} = \nu \left[ \int f_m d\vec{v} - \int f d\vec{v} \right] \\ &= \nu(n - n) = 0 \quad ;\end{aligned}$$

$$\begin{aligned}\Delta(m\mathcal{A}_i) &= m\nu \int \mathcal{A}_i (f_m - f) d\vec{v} \\ &= m\nu \left[ \int \mathcal{A}_i f_m d\vec{v} - \int \mathcal{A}_i f d\vec{v} \right] \\ &= m\nu [0 - \langle \mathcal{A}_i \rangle] = 0\end{aligned}$$

(since  $\langle \mathcal{A}_i \rangle$  is zero):

$$\begin{aligned}\Delta\left(\frac{1}{2}m\mathcal{A}^2\right) &= \nu \left[ \int \frac{1}{2}m\mathcal{A}^2 f_m d\vec{v} - \int \frac{1}{2}m\mathcal{A}^2 f d\vec{v} \right] \\ &= \nu \left( \frac{3}{2}kT - \frac{3}{2}kT \right) = 0 \quad .\end{aligned}$$

The collision terms for the stress and heat flux using the Krook model differ considerably from that obtained for 13-moment theory. Using the Krook model (Eq. (6.5)) we get the following relations:

$$\Delta(m\mathcal{A}_i\mathcal{A}_j) = -\nu P_{ij} \quad , \quad (7)$$

$$\Delta\left(\mathcal{A}_i\frac{1}{2}m\mathcal{A}^2\right) = -\nu q_i \quad . \quad (8)$$

Whereas, using the exact expression for the collision integral, and the 13-moment approximation, one would obtain :

$$\Delta(m v_i v_j) = -\frac{\lambda^2 I}{20} P_{ij} = -\frac{p}{\mu} P_{ij}, \quad (9)$$

$$\Delta(v_i \frac{1}{2} m v^2) = -\frac{\lambda^2 I}{30} q_i = -\frac{5k p}{2m\lambda} q_i, \quad (10)$$

where  $P_{ij}$  are the elements of the stress tensor;  $q_i$  is the  $i^{\text{th}}$  component of the heat flux;  $p$  is the pressure; and  $\mu$  is viscosity of the gas. Comparing Eqs. (7)-(10) we see that the Krook model cannot correctly represent both the stress and heat flux terms. In other words,  $\nu$  in the Krook model can only be chosen to represent either the stress or heat flux terms correctly, but not both. For example we could set:

$$\nu = \frac{\lambda^2 I}{20} = \frac{p}{\mu}; \quad (11)$$

and in this case, Eq. (7) would agree with Eq. (9); but Eqs. (8) and (10) would be off by a factor of 3/2. The fact that both the stress and heat flux cannot correctly be represented at the same time is the biggest shortcoming of the model. We can correct this deficiency by going to a more elaborate model to be discussed below.

#### B. Relaxation properties of the Krook model

If we consider a spatially homogeneous system, so that  $f$  is not a function of  $\vec{x}$ , then Eq. (1) can be written in the form

$$\frac{\partial f}{\partial t} = \nu (f_m - f). \quad (12)$$

Also, spatial homogeneity means  $n$ ,  $\vec{u}$ , and  $\tau$  are constants. Therefore,  $f_m$  is no longer a function of time. This fact makes the integration of Eq. (12) a simple task. Upon carrying out the integration, we obtain

$$f(\vec{v}, t) = f_m(\vec{v}) + [f_m(\vec{v}) - f(\vec{v}, 0)]e^{-\nu t}. \quad (13)$$

This shows that any initial non-equilibrium distribution,  $f(\vec{v}, 0)$ , will relax to the Maxwellian distribution,  $f_m(\vec{v})$ , in a time of the order of magnitude of  $\nu^{-1}$ . This fact, along with Eq. (11), indicates that  $\nu$  is a quantity of the order of magnitude of the collision frequency.

### C. Linearized form of the Krook model

For the case of sound propagation, all the gas properties deviate only slightly from their constant and uniform equilibrium (or ambient) values. We will denote these ambient values by a subscript, zero, and consider small perturbations, or deviations, of all the gas quantities from these ambient values. Thus, we take

$$f = f_0(1 + \phi), \quad (14)$$

$$n = n_0(1 + n'), \quad (15)$$

$$\vec{u} = \vec{u}', \quad (16)$$

$$\tau = \tau_0(1 + \tau'), \quad (17)$$

where  $f_0$ ,  $n_0$ , and  $T_0$  are all constants; the quantities  $\phi$ ,  $n'$ , and  $T'$  are all dimensionless and assumed to be much smaller than unity;  $u'$  is very small in comparison with the average molecular speed; the primed quantities are the departures from the equilibrium value; the quantities  $\phi$ ,  $n'$ ,  $\vec{u}'$ , and  $T'$  are all functions of  $\vec{x}$ , and  $t$ ; whereas  $f_0$  is a function of  $\vec{v}$  only and is defined by

$$f_0 = n_0 \left( \frac{\lambda_0}{\pi} \right)^{3/2} e^{-\lambda_0 v^2}, \quad (18)$$

where

$$\lambda_0 = \frac{m}{2kT_0}.$$

Upon substitution of Eqs. (14)-(17) into Eqs. (1), (3), (5), and (6) we arrive at the following set of equations:

$$n' = \frac{1}{n_0} \int f_0 \phi d\vec{v}, \quad (19)$$

$$\vec{u}' = \frac{1}{n_0} \int \vec{v} f_0 \phi d\vec{v}, \quad (20)$$

$$T' = \frac{2}{3n_0 k T_0} \int \left( \frac{1}{2} m v^2 - \frac{3}{2} k T_0 \right) f_0 \phi d\vec{v}, \quad (21)$$

where the perturbation  $\phi$  is our new unknown. Starting with Eqs. (15) and (17), expanding  $(1 + T)^{-1}$  and neglecting higher order terms, we arrive at the following equation:

$$f_m(\vec{x}, \vec{v}, t) = f_0(\vec{v}) \left[ 1 + n' + T'(\lambda_0 v^2 - \frac{3}{2}) + 2\lambda_0 \vec{u}' \cdot \vec{v} \right]. \quad (22)$$

Also, upon substitution of Eq. (15) into Eq. (1) we obtain

$$f_0 \left[ \frac{\partial \phi}{\partial t} + \vec{v} \cdot \nabla \phi \right] = \nu \left[ f_m - f_0 - f_0 \phi \right]. \quad (23)$$

And by substituting Eq. (22) into Eq. (23) we get

$$\frac{\partial \phi}{\partial t} + \vec{v} \cdot \nabla \phi = \nu \left[ -\phi + n' + \tau' (\lambda_0 v^2 - 3/2) + 2\lambda_0 \vec{u}' \cdot \vec{v} \right]. \quad (24)$$

We can write Eqs. (19), (20), (21), and (24) in semi-dimensionless form by introducing the dimensionless velocity,

$$\vec{c} = \frac{\vec{v}}{\left(\frac{\kappa T_0}{m}\right)^{1/2}} = (2\lambda_0)^{1/2} \vec{v}, \quad (25)$$

where  $\left(\frac{\kappa T_0}{m}\right)^{1/2}$  has the dimension of velocity. Upon substitution of Eq. (25) into Eqs. (24), (18), (19), (20), and (21) we arrive at the following semi-dimensionless equations:

$$\frac{\partial \phi}{\partial t} + (2\lambda_0)^{-1/2} \vec{c} \cdot \nabla \phi = \nu \left[ -\phi + n' + \tau' \left( \frac{1}{2} c^2 - \frac{3}{2} \right) + \vec{w} \cdot \vec{c} \right], \quad (26)$$

where  $\vec{w} = (2\lambda_0)^{1/2} \vec{u}'$ , (26.5)

$$n' = (2\pi)^{-3/2} \int e^{-c^2/2} \phi d\vec{c}, \quad (27)$$

$$\vec{w} = (2\pi)^{-3/2} \int \vec{c} e^{-c^2/2} \phi d\vec{c}, \quad (28)$$

$$\tau' = (2\pi)^{-3/2} \int \left( \frac{1}{3} c^2 - 1 \right) e^{-c^2/2} \phi d\vec{c}. \quad (29)$$

For a one dimensional problem such as sound propagation in the x-direction, Eq. (26) can be written as

$$\frac{\partial \phi}{\partial t} + (2\lambda_0)^{-1/2} c_x \frac{\partial \phi}{\partial x} = \nu \left[ -\phi + n' + \tau' \left( \frac{1}{2} c^2 - \frac{3}{2} \right) + w_x c_x \right] . \quad (30)$$

This equation is known as Linearized Krook model. In order to study the problem of sound propagation in a simple gas, we assume plane wave solutions to Eqs. (27)-(29) of the form

$$\phi(x, \vec{c}, t) = \bar{\phi}(\vec{c}) e^{i(\omega t - kx)} , \quad (31)$$

where  $\omega$  is the frequency of the wave, and  $k$  is the complex wave number and is defined by

$$k = \frac{\omega}{c} - i\alpha , \quad (31a)$$

where  $c$  is the speed of the wave and  $\alpha$  is the absorption coefficient. Upon substituting Eq. (31a) into Eq. (31) we get

$$\begin{aligned} \phi(x, \vec{c}, t) &= \bar{\phi} e^{i[\omega t - (\frac{\omega}{c} - i\alpha)x]} \\ &= \bar{\phi} e^{-\alpha x} e^{i\omega(t - x/c)} , \end{aligned}$$

which shows that the amplitude decreases exponentially with  $x$ , and also that there will not be any absorption unless  $k$  is a complex number. Usually  $\alpha$  and  $c$  are not plotted as a function

of  $\omega$ , but the dimensionless quantities  $\alpha c_0/\omega$  and  $c_0/c$  are plotted as a function of  $\kappa$ . Therefore, Eq. (31a) is rewritten in dimensionless form

$$\kappa c_0/\omega = c_0/c - i\alpha c_0/\omega,$$

$$\text{or} \quad K = c_0/c - i\alpha c_0/\omega, \quad (32)$$

$$\text{where} \quad \kappa = \frac{\omega}{c_0} K. \quad (33)$$

Upon substitution of Eq. (31) into Eqs. (27)-(29), we obtain

$$n'(x,t) = \bar{n} e^{i(\omega t - \kappa x)}, \quad (34)$$

$$w_x(x,t) = \bar{w}_x e^{i(\omega t - \kappa x)}, \quad (35)$$

$$T'(x,t) = \bar{T} e^{i(\omega t - \kappa x)}, \quad (36)$$

$$\text{where} \quad \bar{n} = (2\pi)^{-3/2} \int e^{-c^2/2} \bar{\phi} d\vec{c}, \quad (37)$$

$$\bar{w}_x = (2\pi)^{-3/2} \int c_x e^{-c^2/2} \bar{\phi} d\vec{c}, \quad (38)$$

$$\bar{T} = (2\pi)^{-3/2} \int \left(\frac{1}{3}c^2 - 1\right) e^{-c^2/2} \bar{\phi} d\vec{c}. \quad (39)$$

And by substituting Eq. (31), and Eq. (34)-(36) into Eq. (30) we get

$$\left[ i\omega - (2\lambda_0)^{-1/2} i\kappa c_x + \nu \right] \bar{\phi} = \nu \left[ \bar{n} + \bar{T} \left( \frac{1}{3}c^2 - \frac{3}{2} \right) + \bar{w}_x c_x \right]. \quad (40)$$

By introducing the quantity,

$$\xi = \frac{(2\lambda_0)^{1/2}}{i\kappa} (i\omega + \nu), \quad (41)$$

we can write Eq. (40) in the form

$$(c_x - \xi) \bar{\phi} = \frac{i(2\lambda_0)^{1/2}}{\kappa} \nu \left[ \bar{n} + \bar{\tau} \left( \frac{1}{2} c^2 - \frac{3}{2} \right) + \bar{\omega}_x c_x \right]. \quad (42)$$

Upon substitution of Eq. (33) into Eq. (42), and assuming that  $(c_x - \xi) \neq 0$  we arrive at the following equation for  $\bar{\phi}$ :

$$\bar{\phi} = \left( \frac{5}{3} \right)^{1/2} \frac{1}{\kappa} \frac{i\nu}{\omega} \frac{1}{c_x - \xi} \left[ \bar{n} + \bar{\omega}_x c_x + \bar{\tau} \left( \frac{1}{2} c^2 - \frac{3}{2} \right) \right]. \quad (43)$$

By substituting Eq. (43) into Eqs. (37)-(39) we will get three homogeneous equations in terms of three unknowns, i.e.  $\bar{n}$ ,  $\bar{\omega}$ , and  $\bar{\tau}$ . Then, by setting the determinant of the coefficients to zero we will obtain the dispersion relation. In order to calculate the absorption and dispersion of the sound wave we need the dispersion relation, which in turn will provide us an expression of  $\kappa$  as a function of the rarefaction parameter  $\kappa = \frac{\nu}{\omega}$ . In doing this, for convenience, we invoke a new function of  $\xi$  which is written as

$$G[\xi(\bar{c})] = (2\pi)^{-3/2} \int \frac{\xi(\bar{c}) e^{-\bar{c}^2/2}}{c_x - \xi} d\bar{c}. \quad (44)$$

Now by substituting Eq. (43) into Eqs. (37)-(39) we arrive at the following set of equations:

$$\bar{n} = \left(\frac{5}{3}\right)^{1/2} \frac{1}{K} \frac{i\nu}{\omega} \left[ \bar{n} G(1) + \bar{w}_x G(c_x) + \bar{T} G\left(\frac{1}{2}c^2 - \frac{3}{2}\right) \right],$$

$$\bar{w}_x = \left(\frac{5}{3}\right)^{1/2} \frac{1}{K} \frac{i\nu}{\omega} \left[ \bar{n} G(c_x) + \bar{w}_x G(c_x^2) + \bar{T} G\left[c_x\left(\frac{1}{2}c^2 - \frac{3}{2}\right)\right] \right],$$

$$\bar{T} = \left(\frac{5}{3}\right)^{1/2} \frac{1}{K} \frac{i\nu}{\omega} \left[ \bar{n} G\left(\frac{1}{3}c^2 - 1\right) + \bar{w}_x G\left[c_x\left(\frac{1}{2}c^2 - 1\right)\right] + \bar{T} G\left[\left(\frac{1}{3}c^2 - 1\right)\left(\frac{1}{2}c^2 - \frac{3}{2}\right)\right] \right].$$

These equations can be put in the form of a matrix equation

$$y = Cy, \quad (45)$$

where

$$y = \begin{bmatrix} \bar{n} \\ \bar{w}_x \\ \bar{T} \end{bmatrix}, \quad (46)$$

and

$$C = \left(\frac{5}{3}\right)^{1/2} \frac{1}{K} \frac{i\nu}{\omega} D, \quad (47)$$

where D is a complex matrix and is given by

$$D = \begin{bmatrix} G(1) & G(c_x) & G\left(\frac{1}{2}c^2 - \frac{3}{2}\right) \\ G(c_x) & G(c_x^2) & G\left[c_x\left(\frac{1}{2}c^2 - \frac{3}{2}\right)\right] \\ G\left(\frac{1}{2}c^2 - 1\right) & G\left[c_x\left(\frac{1}{3}c^2 - 1\right)\right] & G\left[\left(\frac{1}{3}c^2 - 1\right)\left(\frac{1}{2}c^2 - \frac{3}{2}\right)\right] \end{bmatrix}.$$

Eq. (45) can be rewritten as

$$(I - C)y = 0.$$

Therefore, the required dispersion relation will be

$$\det(I - c) = |I - c| = 0 \quad .$$

For computational convenience, the matrix equation, Eq. (45) is written in an eigenvalue-eigenvector form. To accomplish this following steps are taken. Eq. (47) can be put into the form

$$C = \left(\frac{5}{3}\right)^{1/2} \frac{1}{K} i\pi D, \quad (48)$$

and by substituting Eq. (48) into Eq. (45) we get

$$\left(\frac{5}{3}\right)^{1/2} \frac{1}{K} i\pi D y = y. \quad (49)$$

But upon substitution of Eq. (41) into Eq. (40) we obtain

$$\xi = \left(\frac{5}{3}\right)^{1/2} \frac{1}{K} (1 - i\pi), \quad (50)$$

or equivalently,

$$K = \left(\frac{5}{3}\right)^{1/2} \frac{1 - i\pi}{\xi}. \quad (51)$$

Therefore Eq. (49) can be written as

$$\xi D y = \left(\frac{1 - i\pi}{i\pi}\right) y,$$

also, introducing a new matrix A such as  $A = \xi D$  the above equation can be rewritten as

$$A y = -\left(1 + \frac{i}{\pi}\right) y. \quad (52)$$

Eq. (52) is of the form of the general eigenvalue-eigenvector equation, viz.,

$$AY = \lambda Y, \quad (53)$$

where  $y$  is the eigenvector, and  $\lambda$  is the eigenvalue given by

$$\lambda = -\left(1 + \frac{i}{\pi}\right). \quad (54)$$

The matrix elements of  $D$  are given by

$$D_{11} = F(\xi),$$

$$D_{12} = 1 + \xi F(\xi),$$

$$D_{13} = \frac{1}{2}\xi + (\xi^2 - 1)F(\xi),$$

$$D_{21} = 1 + \xi F(\xi),$$

$$D_{22} = \xi [1 + \xi F(\xi)],$$

$$D_{23} = \frac{1}{2} [\xi + (\xi^2 - 1)F(\xi)],$$

$$D_{31} = \frac{1}{3} [\xi + (\xi^2 - 1)F(\xi)],$$

$$D_{32} = \frac{1}{3}\xi [\xi + (\xi^2 - 1)F(\xi)],$$

$$D_{33} = \frac{1}{6} [\xi^2 - \xi + (\xi^4 - 2\xi^2 + 5)F(\xi)],$$

where  $F(\xi)$  is a new function of  $\xi$  and is given<sup>7</sup> by

$$F(\xi) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \frac{e^{-c_x^2/2}}{c_x - \xi} dc_x.$$

As can easily be seen, it would be a hard task to solve the equations analytically, so we therefore rely upon the computer and numerical methods. What is sought is the solution of the equations for the  $\lambda$ 's. We start with a fixed value of  $\text{Im}(\xi)$  and vary the value of  $\text{Re}(\xi)$ . Each time the computer finds the elements of matrix A and solves for  $\lambda$ . The value of  $\text{Re}(\xi)$  is continuously varied until we get a purely imaginary value of the quantity,  $-(\lambda+1)$ . If Eq. (54) is written as

$$-(\lambda+1) = \frac{i}{\kappa}, \quad (55)$$

then the reciprocal of the above obtained value is equal to  $\kappa$ . Therefore, by substituting the value of  $\kappa$  and  $\xi$  into Eq. (51) we can get the value of K of which the real and imaginary parts, as seen from Eq. (32), are the dispersion and absorption respectively. Therefore, we can calculate the absorption and dispersion of the sound wave by solving the Eq. (53).

CHAPTER III  
NUMERICAL METHODS

Our motivation is to duplicate the results obtained by Sirovich and Thurber<sup>3</sup> for a sound wave propagating through a simple monatomic gas. Once we duplicate the results for a simple gas then by changing the order of the matrix we can use the same program for a mixture of gases. We wish to calculate the absorption and dispersion of the sound wave using the Krook model and compare the results with the values obtained by Sirovich and Thurber.

In the previous chapter, Eq. (32) tells us that the absorption,  $\alpha c_0/\omega$ , is the negative imaginary part of  $K$  and the dispersion,  $c_0/c$ , is the real part of  $K$ . From Eq. (51), we had

$$K = \left(\frac{5}{3}\right)^{1/2} \frac{1 - i\kappa}{\xi} ;$$

therefore, we want to find out some way which would give us the corresponding values of  $\kappa$  and  $\xi$ , which in turn will give us one value of  $K$ . That is one value of  $K$  could be obtained from a pair of  $\kappa$  and  $\xi$ .

Our first step is to draw a root trajectory in the complex  $\xi$ -plane. We find the values of real  $K$  and the negative of imaginary  $K$  corresponding to different values of  $\kappa$  from the graphs drawn by Sirovich and Thurber. On

substitution of these values, i.e.,  $K$  and  $\kappa$  into Eq. (51) the real and imaginary part of  $\xi$  can be obtained. In other words for a given  $\kappa$  and for the given values of real and imaginary  $K$ , obtained from the graphs, we could get a corresponding  $\xi$ . So the root trajectory in  $\xi$ -plane, which is a graph of  $\text{Im}(\xi)$  versus  $\text{Re}(\xi)$ , can be plotted. The trajectory gives us an approximate value of real  $\xi$  for a fixed value of imaginary  $\xi$ .

Referring to Eq. (53), we observe that  $A$  is a complex matrix; and all elements can be expressed as a function of  $F(\xi)$ . For different values of  $\xi$ ,  $F(\xi)$  can be obtained by the subroutine FCAL<sup>8</sup>. Using the value of  $F(\xi)$  we can get the elements of matrix  $A$ . We wish to solve Eq. (53) to obtain the eigenvalues and eigenvectors. We use the subroutine called DCOMEIG<sup>9</sup>, which solves eigenvalue equation for any complex square matrix of any order and gives the corresponding eigenvalues and eigenvectors.

Finally, we develop a PL/1 computer program which solves the eigenvalue equation and calculates  $\kappa$  and  $\xi$  simultaneously, which in turn can give us different values of  $K$ . This program has two subroutines, one called MAT<sup>10</sup>, and the other called DECOMEIG. The former calculates the matrix elements of  $A$  with the help of the function subprogram FCAL; whereas, the latter solves the eigenvalue equation as explained earlier. To obtain a pair of  $\kappa$  and  $\xi$ , we fix

the imaginary  $\xi$  and vary real  $\xi$  in a range which can be guessed from the root trajectory in complex  $\xi$ -plane. For each value of real  $\xi$  the subroutines MAT and DECOMEIG are called. DECOMEIG gives us the complex eigenvalues ( $\lambda$ ) and the corresponding eigenvectors. For a simple gas, A is a square matrix of order three. Thus, we get three eigenvalues and three eigenvectors. In order to check which of these eigenvalues are of interest we compute the value of the quantity,  $(\lambda + 1) = X$ , for different values of real  $\xi$  in the range chosen, for the fixed imaginary  $\xi$ . If the sign of the real part of X changes, then the corresponding eigenvalues are of interest. Observing Eq. (55) we can say that for these (above mentioned) eigenvalues the real part of X must vanish for a value of real  $\xi$  as we move along a straight line parallel to the axis of real  $\xi$ . In other words we wish to find the value of real  $\xi$  for which X is purely imaginary. We do this by following the method of bisection. If the real part of X gets very, very small compared to its imaginary part, then the imaginary part of X is approximately equal to  $1/\kappa$ . Therefore, the inverse of the imaginary part is approximately equal to  $\kappa$ .

The value of real  $\xi$ , for which X is purely imaginary, together with the value of fixed imaginary  $\xi$  gives us a point on complex  $\xi$  plane corresponding to the  $\kappa$  just obtained above. By fixing a new value of imaginary  $\xi$  and

then following the same procedure we could get a second pair of  $\xi$ , and  $\kappa$ , and so on. Each pair of  $\xi$  and  $\kappa$  gives us a new value of  $K$ . As mentioned earlier, the real part of  $K$  is the dispersion, and the negative imaginary part of  $K$  is the absorption, of the sound wave. Both the absorption and dispersion are expressed as a function of  $\kappa$ . This is because we want to compare the theoretical results with the experimental data; and in experiments it is customary to measure the absorption and dispersion of the sound wave as a function of the rarefaction parameter,  $\kappa$ . The output of the final program contains values of  $\text{Im}(\xi)$ ,  $\text{Re}(\xi)$ ,  $\kappa$ , the eigenvalues, the eigenvectors,  $\text{Re}(K)$ , and  $\text{Im}(K)$ . Hence, we can draw the graphs of the real part of  $K$  versus  $\kappa$ , and the negative imaginary part of  $K$  versus  $\kappa$ . These graphs can be compared with those obtained by Sirovich and Thurber. The agreement of the former graphs with the latter one verifies the computer program. Some possible difficulties which may be encountered in drawing graphs of the absorption and dispersion versus  $\kappa$  are discussed below.

The first problem is to decide which one of the three eigenvalues gives the true values of the absorption and dispersion. In other words, which eigenvalue yields the right value of  $\kappa$ . In most cases when the value of real  $\xi$  is varied in the known range, the sign changes for  $X$  only for one of the three eigenvalues. No complications arise in

this case; but if the sign of  $X$  changes for more than one eigenvalue then it will be a hard task to decide which eigenvalue would give the right value of  $\kappa$ .

The dispersion relation has three solutions. Out of these three solutions only one corresponds to the absorption and dispersion of sound. All points obtained from the three solutions should be plotted in absorption and dispersion graphs. We know the values of absorption and dispersion at  $\kappa=0$ , and 100 from the graphs drawn by Sirovich. This information helps us in drawing the graph. If the set of points obtained from one solution are far away from other points obtained from other solution then by observing the points we can draw the right curve. But, if two sets of points obtained from two solutions overlap then the following two cases may arise.

a) Figure (1) shows two sets of points crossing at one point (B). Different curves could be drawn through these points. But we know that the absorption and dispersion curves are smooth curve. Therefore, either AC or DE would be the right curve. But, we know the value of  $c_0/c$  at  $\kappa=0$ , and 100. Hence, we would be able to draw the dispersion curve without any ambiguity.

b) In this case (Fig. (2)) two sets of points are tangent to each other. To avoid this difficulty we can check the value of  $\kappa$  more precisely. We can change the interval of

$\text{Re}(\xi)$  to a very small value and we might get two different values of  $\xi$  for the same  $\lambda$ . Therefore, the two sets of points will not be tangent to each other. But if we still find the sets of points as tangent to each other, then we can check the behaviour of the eigenvectors along each curve. The curve along which the values of the eigenvectors change smoothly is the true one.

At first we worked with each subroutine separately. After much arrangements we found that each subroutine was functioning properly. That is, each of them gave the correct results. Therefore, we wanted to write a driving program for calculating the absorption and dispersion of sound which would include all subroutines, i.e., MAT, FCAL, and DECOMEIG. We developed the final program but, the sign did not change for the eigenvalues. Much efforts were put to duplicate Sirovich's results. Several programs were written but due to some minor error in the driving program we could not get the change of sign for the eigenvalues as was expected. Therefore, we conclude that some more work has to be done in order to get the final results.

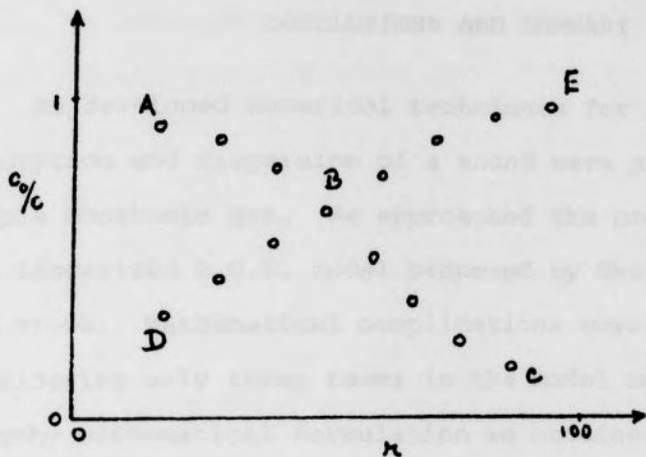


Figure 1: The plot of the dispersion versus the rarefaction factor. The curves are crossing at one point but not tangent to each other.

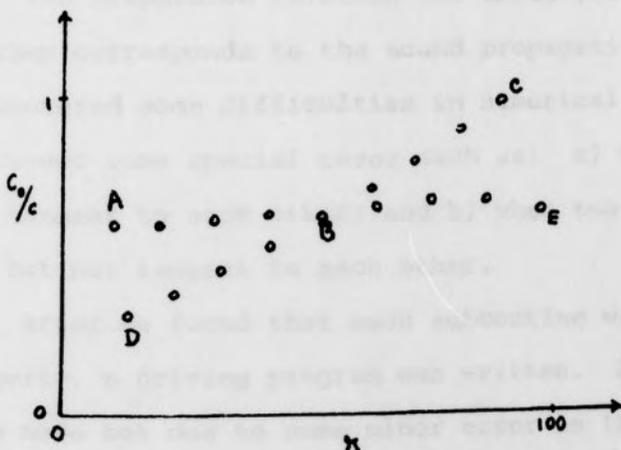


Figure 2: Plot of the dispersion versus the rarefaction factor. The curves are tangent to each other.

## CONCLUSIONS AND SUMMARY

We developed numerical techniques for the study of the absorption and dispersion of a sound wave propagating in a simple monatomic gas. We approached the problem by using the Linearized B.G.K. model proposed by Bhatnagar, Gross, and Krook. Mathematical complications were decreased by considering only three terms in the model equation. After lengthy mathematical formulation we obtained a set of linear equations in the general eigenvalue-eigenvector form. The solution of this yields the absorption and dispersion in terms of the rarefaction parameter. Numerical methods were discussed for solving the eigenvalue equation and for developing a PL/1 computer program for calculating the absorption and dispersion of sound.

The dispersion relation has three solutions, and one of them corresponds to the sound propagation. Therefore, we encountered some difficulties in numerical analysis. We discussed some special cases such as: a) when two curves are tangent to each other; and b) when two curves are crossing but not tangent to each other.

After we found that each subroutine was functioning properly, a driving program was written. Several attempts were made but due to some minor error in the final program



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## APPENDIX I

## Program Listing

```

*PROCESS;
MAT: PROC(TSI,C);
/* THIS A SUBROUTINE (NOT A FUNCTION) WHICH CALCULATES THE MATRIX */
/* C GIVEN TSI. */
DCL (F,TSI) BIN FLOAT(53) CPLX,
C(*,*)BIN FLOAT(53)COMPLEX;
DCL FCAL ENTRY(BIN FLOAT(53) CPLX) RETURNS(BIN FLOAT(53) CPLX);
F=FCAL(TSI);
PUT DATA(F);
C(1,1)=F;
C(1,2)=1+TSI*F;
C(2,1)=C(1,2);
C(1,3)=(TSI+(TSI**2=1)*F)/2;
C(2,2)=TSI*C(1,2);
C(2,3)=TSI*C(1,3);
C(3,1)=2*C(1,3)/3;
C(3,2)=TSI*C(3,1);
C(3,3)=(TSI**3-TSI+(TSI**4-2*TSI**2+5)*F)/6;
C=TSI*C;
RETURN;
END MAT;
*PROCESS;
FCAL:PROC(TSI) RETURNS(BIN FLOAT(53) CPLX);
DCL(DUMA,DUMB,DUMC,DIUMD) BIN FLOAT(53);
DCL(A(0:100),B(0:100)) BIN FLOAT(53) CPLX;
DCL(SUMA,SUMB,LSUMA,LSUMB) BIN FLOAT(53) INIT(0);
DCL(XZ,YZ,LXZ,LYZ) BIN FLOAT(53) INIT(0);
DCL(SQTPI,AX,AY,BX,YB,S1,S2,S3,S4,W) BIN FLOAT(53);
DCL(ZNEG,TSI,TSIP,7,INT,SA,SB) BIN FLOAT(53) CPLX;
DCL F BIN FLOAT(53) CPLX;
DCL(DELX,DELY,SQT_TWO) BIN FLOAT(53);
SQTPI=1.772453850;
SQT_TWO=1.414213562;
TSI=TSI/SQT_TWO;
IF REAL(TSI)=0 THEN DO;
Z=SQTPI*EXP(YB**2)*ERFC(YB)*1I;
GO TO OVER;
END;
TSIP=TSI;
IF IMAG(TSI)=0 THEN DO;
Z=(1I-ERF(BX))*SQTPI/EXP(BX**2);
GO TO OVER;
END;
/*
/*

```

```

/*          NUMERICAL INTERGRATION          */
/*                                          */
/*                                          */
/* IF ABS(IMAG(TSIP))<2 THEN DO;          */
AX,AY=0;
RX=REAL(TSIP);
YB=IMAG(TSIP);
N2=1+ABS(BX=AX)/.01;
N=2*N2;
H=(BX-AX)/FLOAT(N,16);
S1=FA(AX,AY)+4.*FA((AX+H),AY);
S2=FB(AX,AY)+4.*FB((AX+H),AY);
L1: DO I=1 TO N2-1;
DUMA=AX+H*(2*I);
DUMB=AX+H*(2*I+1);
S1=S1+2.*FA(DUMA,AY)+4.*FA(DUMB,AY);
S2=S2+2.*FB(DUMA,AY)+4.*FB(DUMB,AY);
END L1;
S1=H*(FA(BX,AY)+S1)/3;
S2=H*(FB(BX,AY)+S2)/3;
N2=1+ABS(YB=AY)/.01;
N=2*N2;
H=(YB-AY)/FLOAT(N,16);
S3=FC(BX,AY)+4.*FC(BX,(AY+H));
S4=FD(RX,AY)+4.*FD(BX,(AY+H));
L2: DO I=1 TO N2-1;
DUMC=AY+H*(2*I);
DUMD=AY+H*(2*I+1);
S3=S3+2.*FC(BX,DUMC)+4.*FC(BX,DUMD);
S4=S4+2.*FD(BX,DUMC)+4.*FD(BX,DUMD);
END L2;
S3=H*(FC(BX,YB)+S3)/3.;
S4=H*(FD(BX,YB)+S4)/3.;
INT=S1/EXP(AY**2)-EXP(RX**2)*S4+(S2/EXP(AY**2)+EXP(RX**2)*S3)*I;
Z=(SQTP1*I=2*INT)/EXP(TSIP**2);
END;
ELSE DO;
/*                                          */
/*                                          */
/*          ASYMPTOTIC EXPANSION          */
/*                                          */
/*                                          */
DELX,DFLY=1;
A(1)=1;
A(0)=0;
B(0)=1;
R(1)=2*TSIP;
FRAC: DO N=1 TO 99 WHILE (DELX>1.0E-15 I DFLY>1.0E-15);
A(N+1)=(2*TSIP*A(N)-2*N*A(N-1));
B(N+1)=(2*TSIP*B(N)-2*N*B(N-1));
Z=2*A(N+1)/B(N+1);
XZ=REAL(Z);
YZ=IMAG(Z);

```

```

      DELX=ABS((IXZ-XZ)/XZ);
      DELY=ABS((IYZ-YZ)/YZ);
      LXZ=XZ;
      LYZ=YZ;
      END FRAC;
IF IMAG (TSI)>0 THEN DO;
Z=Z-2I*SQTP1*EXP(-TSI**2);
END;
      END;
OVER: F=Z/SQT_TWO;
      RETURN(F);
FA: PROC(X,Y) RETURNS(BIN FLOAT(53));
      DCL(X,Y,C1) BIN FLOAT(53);
      IF X**2>174 THEN
LA: DO;
      RETURN(0);
      END LA;
      ELSE DO;
      C1=EXP(X**2)*COS(2*X*Y);
      RETURN(C1);
      END;
      END FA;
FB: PROC(X,Y) RETURNS(BIN FLOAT(53));
      DCL(X,Y,C2) BIN FLOAT(53);
      IF X**2>174 THEN
LR: DO;
      RETURN(0);
      END LB;
      ELSE DO;
      C2=EXP(X**2)*SIN(2*X*Y);
      RETURN(C2);
      END;
      END FB;
FC: PROC(X,Y) RETURNS(BIN FLOAT(53));
      DCL(X,Y,C3) BIN FLOAT(53);
      C3=COS(2*X*Y)/EXP(Y**2);
      RETURN(C3);
      END FC;
FD: PROC(X,Y) RETURNS(BIN FLOAT(53));
      DCL(X,Y,C4) BIN FLOAT(53);
      C4=SIN(2*X*Y)/EXP(Y**2);
      RETURN(C4);
      END FD;
      END FCAL;

```