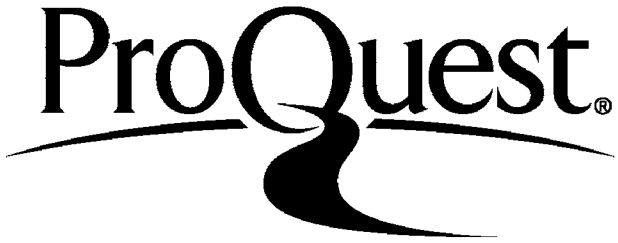
" SOLUBLE IDEALISED MODELS IN PARTICLE TRANSPORT THEORY "

RAVAL. SHASHIKANT

A THESIS SUBMITTED FOR THE DEGREE OF DOCTOR OF PHILOSOPHY IN THE UNIVERSITY OF LONDON.

DEPARTMENT OF PHYSICS,
BEDFORD COLLEGE,
REGENT'S PARK,
LONDON NW1 4NS.



Abstract

The central aim of Part I of this thesis is to investigate non-equlibrium processes in physics by studying the so called Rayleigh's Piston model which was originally conceived by Lord Rayleigh in 1891. In its most general aspect the modern formulation involved the study of the 'Master Equation' for the statistical evolution of an ensemble of test-particles (mass M) constrained to move in one dimension interacting with heat-bath particles (mass m). By using the numerical techniques developed in studying neutron thermalisation, we have investigated the accuracy of Rayleigh's original treatment or the so called Brownian limit and obtained numerical results for velocity autocorrelation function $S_V(t)$ and electrical conductivity $\sigma(\omega)$.

It is in the case of special Rayleigh's model where the masses are equal (M=m) that we have been able to solve the model exactly both by using the method of singular eigenfunctions and by the method of Laplace transform. Thus a definitive connection is made with methods developed in the 'Linear Transport Theory' to solve problems in field of radiative transfer, neutron diffusion, the theory of plasma as well as elsewhere. For the special model, we have investigated the 'Velocity' barrier problem, the spatial problem and obtained exact expressions for the autocorrelation function, the diffusion constant, the electrical conductivity by using the linear response theory and tested the validity of the so called 'Gaussian Approximation' by examining moments of the Van Hove correlation function $G(r,t)$.

In Part II of this thesis we have investigated the behaviour of a model consisting of an ideal charged electron gas in a uniform magnetic field and confined by a cylinderically symmetric potential. We have obtained exact expressions for the current density, the magnetic moment, the magnetic susceptibility and examined in detail the boundary effects.

Acknowledgements

It is a pleasure to record my gratitude to all the following.

Dr. M.R. Hoare for supervising Part I of this thesis.
Dr. M. Rahman whose advice and valuable comments have been both stimulating and helpful to me.
Dr. B.U. Felderhof for supervising Part II of this thesis.
Dr. J.A. Barker for his collaboration.

Finally, I want to record gratefully that this work has been partially supported by the Science Research Council.

to Tanuja

CONTENTS

PART I

' Of what use is your beautiful investigation regarding pi ? ' (Kronecker to Lindemann)

CHAPTER ONE

INTRODUCTION TO PART I

Section 1.1. Non-equilibrium Physics

The irreversibility of physical processes is the most characteristic feature of the physical world. We know from experience that systems with many degrees of freedom, when left to themselves tend to an equilibrium state which is independent of the initial state. We should in principle be able to handle this problem by solving the Liouville equation, with appropriate initial and boundary conditions. A detailed analysis of the solution should bring out all the features of the macroscopic processes. One is assuming that without modifying the microscopic equations, it would be possible to describe the evolution of the system.

But the elementary laws of motion are reversible, however, the subsequent time evolution of a system is always in a privileged direction. This is the celebrated paradox of irreversibility. The study of the irreversibility problem is beset with enormous difficulties and historically has given rise to many controversies. Failing to deduce the irreversible approach to equilibrium in a systematic way, physicists have attempted to explain the problem from probabilistic considerations. In these treatments, the laws of motion assumed for the individual particles delibrately deviates from the laws of mechanics. At some point in the treatment, an element of probabilistic nature is introduced in the theory.

The earliest and most profound contribution to this problem was made by L.Boltzmann (1872), who gave a probabilistic explanation of the second law of thermodynamics and introduced the H-theorem.

In Part I of this investigation, we have been concerned with the stochastic theory approach to non-equilibrium statistical mechanics. By using physical intuition a workable model of physical systems is constructed where all the ingredients of an irreversible evolution are present. Many problems can be treated by applying this theory. By an exact analysis of the many body problem, it can be shown that in many important cases, the stochastic method can be justified.

The progress in our knowledge of stochastic processes has been quite extensive since Kolmogorov's fundamental paper in 1931. Doubtless as a result of the growing need for the stochastic treatment of problems in diverse fields of modern science. Many parts of the theory were first developed in connection with the study of fluctuations and noise in electric circuits (Schottky 1918). At present, stochastic processes provide models in such diverse fields as the theory of population growth, communication and control theory, operational research and genetics. (see e.g. Bartlett 1962)

Generally the processes in nature are slow and the number of particles very large. Such processes can be treated with advantage as random or stochastic processes. This

approach is semiphenomenological and from the begining a deterministic approach is given up in favour of a more intuitive treatment. In the next section, we have briefly reviewed several general ideas and methods of the theory of stochastic processes (see e.g. Balescu 1975).

Section 1.2. Random Processes

We now come to a definition which plays an important role in many practicle applications. Let y signify the variable in which one is interested. It may be, for example, the current in a noisy electrical circuit. At every given time, y can have random values within its range of variation. To every possible value y at time t we assume a certain probability density; thus $P(y,t)dy$ is a probability of finding the value of the variable in the infinitesimal interval $(y, y+dy)$.

In general the knowledge of the probability density $P(y,t)$ is not sufficient for the characterisation of the process. If it is known that the variable had a value y_1 at t_1, then the probability of finding the value y_2 at t_2 will be influenced by this result because the various values are not necessarily independent. In other words, the correlation between what happens at time t_1 and what happens at time t_2, can best be specified by the 'joint probability density' $P_2(y_2,t_2 \mid y_1,t_1)$ (which is the probability of finding the value y_1 at t_1 and the value y_2 at t_2). The joint probability density cannot generally be inferred from the knowledge of $P_1(y_1,t_1)$.

Therefore, for the complete description, it is necessary to specify all the joint probabilities, $P_1(y_1,t_1)$, $P_2(y_2,t_2 | y_1,t_1)$, and so on, ad infinitum. Clearly, to make further progress, it is necessary to introduce a classification of random processes. The simplest assumption we can make is one in which the knowledge of $P_1(y_1,t_1)$ would suffice for the problem. Namely,

$$P_2(y_2,t_2 | y_1,t_1) = P_1(y_2,t_2).P_1(y_1,t_1) \qquad (1.1)$$

In the above purely random process, correlation in time are completely absent. This is, however, a very unrealistic assumption, particularly for a continous physical process. For short enough time intervals, one would expect to observe a causal relationship between succesive events.

The next simplest case is of fundamental importance in physical applications. The whole information is now contained in the first two distributions. In order to define this process, it is convenient to define a 'transition probability' $W_2(y_2,t_2 | y_1,t_1)$, which is the probability of a transition from y_1 to y_2 in time $t_2 - t_1$. The transition probability is defined through the relationship:

$$P_2(y_2,t_2 | y_1,t_1) = W_2(y_2,t_2 | y_1,t_1).P_1(y_1,t_1) \qquad (1.2)$$

This relationship tells us that the joint probability density equals the probability density of finding y_1 at t_1 times the probability of a transition from y_1 to y_2 in time interval $t_2 - t_1$.

From above the following properties follow quite naturally:

(i) $W_2(y_2,t_2 \mid y_1, t_1) \geqslant 0.$ (1.3)

(ii) $\int dy_2 W_2(y_2,t_2 \quad y_1, t_1) = 1.$ (1.4)

(iii) $P_1(y_2,t_2) = \int dy_1 \, W_2(y_2,t_2 \quad y_1,t_1).P_1(y_1,t_1)$ (1.5)

The $n^{th.}$ order transition probability

$$W_n(y_n, t_n \mid y_1,t_1; y_2,t_2;\ldots\ldots;y_{n-1},t_{n-1})$$

is defined as the 'conditional probability' density of finding the value y_n at time t_n, given that y had the values y_{n-1}, $y_{n-2}, \ldots\ldots\ldots, y_1$ at the times $t_{n-1}, t_{n-2}, \ldots\ldots\ldots, t_1$. The n-successive times are assumed to be ordered:

$$t_1 < t_2 < t_3 \ldots\ldots\ldots t_{n-1} < t_n .$$

A Markov process is defined by the condition :

$$W_n(y_n,t_n \mid y_1,t_1 ;\ldots\ldots;y_{n-1},t_{n-1}) = W_2(y_n,t_n \mid y_{n-1},t_{n-1}) \quad (1.6)$$

This equation implies that for a Markov process, the probability of a transition at time t_{n-1} from y_{n-1} to a value y_n at time t_n depends (besides on y_n, t_n) only on the value of y at time t_{n-1} and not at all on the previous history of the system. It is very easy now to follow through the following steps.

$$P_3(y_3,t_3 \; y_2,t_2;y_1,t_1) = W_3(y_3,t_3 \mid y_2,t_2;y_1, t_1).$$
$$P_2(y_2,t_2 \mid y_1,t_1)$$

$$= W_2(y_3,t_3|\,y_2,t_2).P_2(y_2,t_2|\,y_1,t_1)$$

$$= \frac{P_2(y_3,t_3|\,y_2,t_2).P_2(y_2,t_2|\,y_1,t_1)}{P_1(y_2,t_2)} \qquad (\ 1.7\ )$$

But from the definition of a probability density,

$$P_2(y_3,t_3|\,y_1,t_1) = \int dy_2 P_3(y_3,t_3|\,y_1,t_1;y_2,t_2) \qquad (\ 1.8\ )$$

and from (1.7)

$$P_2(y_3,t_3|\,y_1,t_1) = \int dy_2 W_2(y_3,t_3\ y_2,t_2).W_2(y_2,t_2\ y_1,t_1).P_1(y_1,t_1) \qquad (\ 1.9\ )$$

Combining this with (1.5) we can write

$$W_2(y_3,t_3\ y_1,t_1) = \int dy_2 W_2(y_3,t_3\ y_2,t_2).W_2(y_2,t_2\ y_1,t_1) \qquad (\ 1.10\ )$$

This identity for the 'conditional probabilities' is an integral equation often accepted as a definition of a Markov process. It is called the 'Chapman-Kolmogorov' equation (or sometimes the Smoluchowski equation). The physical interpretation of the above equation is clear. The probability of transition from y_1 at t_1 to y_3 at t_3 can be calculated by taking the product of the probability of transition to some value y_2 at an intermediate time t_2 and the probability of a transition from that value to the final one at t_3 , and integrating over all possible intermediate values.

We have not given further details about the general Markov process and the above identity; the mathematical background is readily accessible (Cox and Miller 1965); this identity forms the basis of most applications of the theory in physics and elsewhere. In control theory it is used to obtain differential-stochastic equations by making further assumptions (Larson 1969).

In order to obtain from the above identity the transport equation for dynamical evolution of the probability distribution $P(y,t)$, further simplifications have to be made. From Chapman-Kolmogorov equation it is possible to derive the Master equation which has formed the basis of this part of the thesis. For pedagogical reasons, the presentation is less deductive than might be desired by a mathematician and only a brief survey of the subject has been presented. Our intention is to present a physically intuitive picture of linear physical processes and not to present long and doubtful calculations, applicable only to a few physical systems. We have therefore, whenever possible, been less concerned with details which are available elsewhere (Felderhof 1961).

let $t_3 = t_2 + \Delta t$ in the above identity. Then

$$W_2(y_3, t_2 + \Delta t | y_1, t_1) = \int dy_2 W_2(y_3, t_2+\Delta t | y_2, t_2) W_2(y_2, t_2 | y_1, t_1) \qquad (1.11)$$

Let us now specialise the discussion to the physically important situation in which the transition probability $W_2(y_2, t_2 | y_1, t_1)$ does not depend on the time t_1 at which the transition occurs, but only on the time interval $t_2 - t_1$.

(As the two-event transition probability W_2 is the only independent transition probability in a Markov process, the subscript 2 is clearly superfluous and can be dropped)

$$W_2(y_2,t_2|y_1,t_1)= W(y_2|y_1;t_2-t_1) \qquad (1.12)$$

For small Δt we can write

$$W(y',t+\Delta t|y,t)= (1-\Delta t\, K(y'|y)dy')\delta(y-y') + \Delta t K(y'|y) + O(\Delta t) \qquad (1.13)$$

The delta term denotes the possibility that no transitions take place and $K(y'|y)$ is the transition probability density per unit time from continuous state y to y'. Therefore $K(y'|y) \geqslant 0$ and for convenience one can define:

$$A(y) = \int dy'\, K(y'|y) \qquad (1.14)$$

By substituting $W(y',t+\Delta t|y,t)$ from (1.13) into (1.11) and taking the limit $\Delta t \longrightarrow 0$, the following differential form of identity (1.10) is obtained :

$$\frac{\partial W}{\partial t}(y_3,t_3|y_1,t_1)= \int dy_2 \left[K(y_3|y_2)W(y_2,t_2|y_1,t_1) - K(y_2|y_3)W(y_3,t_3|y_1\ t_1)\right] \qquad (1.15)$$

By multiplying the above equation throughout by $P_1(x_1,t_1)$ and integrating over y_1 on both sides it follows from (1.2) and (1.5) that:

$$\frac{\partial P(y,t)}{\partial t} = \int dy' K(y|y')P(y',t)-A(y)P(y,t) \qquad (1.16)$$

The Markovian equation (1.16) is the customary form of the Master equation, which relates the evolution of probability distribution P(y,t) in time to the transitions in and out of states. For discrete systems, the Master equation can be written in somewhat familiar form as:

$$\frac{dP_n(t)}{dt} = \sum_{n'} W_{nn'}P_{n'}(t) - W_{n'n}P_n(t) \qquad (1.17)$$

In Quantum Mechanics (1.17) is commonly called the Pauli equation. The first term on the right hand side describes the transitions into a state n, while the second term describes the transitions taking place from state n to any other state n'.

The usefulness of this approach is that the transition probability per unit time K(y'| y) is related to the physical system and for simple models can be computed exactly from the microscopic properties of the system. There are cases in the literature where exact expressions have been obtained for K(y'| y). (see e.g. Alkemade 1956, Van Kampen 1960).

Section 1.3. Properties of the Master equation

By introducing the operator

$$\hat{\omega}(x|x') = K(x|x') - \delta(x-x')A(x)$$

with the definition,

$$\hat{\omega}.P(x,t) = \int dx' K(x|x')P(x',t) - A(x) \qquad (1.18)$$

the Master equation (1.16) follows as,

$$\frac{\partial P(x,t)}{\partial t} = \hat{\omega}.P(x,t) \qquad (1.19)$$

with a formal solution

$$P(x,t) = \exp(\hat{\omega}t).P(x,0) \qquad (1.20)$$

However, the formal solution is of no use in finding the explicit value of $P(x,t)$. The familiar method of solving equations of the type (1.19) by determining the eigenvectors and eigenvalues of $\hat{\omega}$ cannot be used generally because $\hat{\omega}$ need not be symmetric. Thus generally, it is not certain that all solutions can be obtained as superpositions of these eigenvectors.

In the case of a real closed system, one would expect the Master equation to have a unique stationary solution and to satisfy the principle of detailed balance. In this case, $P(x,t)$ after a long time must tend to the equlibrium probability distribution $P_{eq}(x)$ and then it is possible to symmetrise the operator $\hat{\omega}$. Before we discuss the problem of symmetrisation, it is convenient to list all the properties of the Master equation which hold quite generally.

(a) Positivity Condition.

If $P(x,t) \geqslant 0$ at $t=0$ for all values of x then $P(x,t) \geqslant 0$ for all values of x and t;
the proof is quite straightforward(Felderhof 1961)

(b) Uniqueness of Equilibrium

$\lim_{t \longrightarrow 0} P(x,t) = P_{eq}(x)$ for any $P(x,t)$.

Any realistic model has to satisfy this property. In

Appendix A we have presented the proof which is normally proved only for discrete-state systems. (It is important to notice that both (a) and (b) hold irrespective of the nature of eigenvalue spectrum.)

(c) The Principle of detailed balance

For real closed physical systems, it is reasonable to assume that $P_{eq}(x)$ must be the only solution satisfying

$$\int dx' \left[K(x|x') P_{eq}(x') - K(x'|x) P_{eq}(x) \right] \qquad (1.21)$$

In many cases one can make the stronger assertion that the integrand in (1.21) itself vanishes. That is

$$K(x|x') P_{eq}(x) = K(x'|x) P_{eq}(x) \qquad (1.22)$$

The above relationship is a natural symmetry relation for most physical systems (Haken 1975). It can be shown that the detailed balance is a consequence of the invariance of the microscopic equations of motion under time reversal. In case of dynamical variables such as the flow velocity of a fluid, the detailed balance principle reflects the symmetry inherent in the process.

(d) Detailed Balance and Symmetrisation

We can look for the exponential solutions of the Master equation (1.16) of the form:

$$P(x,t) = \exp(-\lambda t) \phi(x,\lambda) \qquad (1.23)$$

where the eigenvalues have been specified by λ and the eigenfunctions by $\phi(x,\lambda)$. Using detailed balance condition (1.22) the operator $\hat{\omega}$ can be symmetrised. The following symmetric kernel can be defined:

$$G(x|x') = K(x|x').N(x')/N(x) \qquad (1.24)$$

where $N(x) = (P_{eq}(x))^{\frac{1}{2}}$ and from (1.22) it follows that:

$$G(x|x') = G(x'|x) \qquad (1.25)$$

This leads immediately to the new self-adjoint Master equation

$$\frac{\partial h(x,t)}{\partial t} = \int dx' G(x|x')h(x',t) - A(x)h(x,t) \qquad (1.26)$$

with $h(x,t) = P(x,t)/N(x)$ (1.27)

In operator form the above equation can be written as

$$\frac{\partial h(x,t)}{\partial t} = \hat{A}.h(x,t) \qquad (1.28)$$

where the operator $\hat{A}$ is defined by the relationship

$$\hat{A} = G(x|x') - A(x)\delta(x-x')$$

In Appendix A it is proved that the operator is negative semi-definite with the consequence that λ the eigenvalues of the symmetrised equation

$$\hat{A}\,\underline{\Phi}(x,\lambda) = -\lambda\,\underline{\Phi}(x,\lambda) \qquad (1.29)$$

are positive. Hence the spectrum of the eigenvalues may be discrete or continuous, or a combination of both but always will lie along the positive real axis. The symmeterised eigenfunctions are related to the eigenfunctions $\phi(x,\lambda)$ of operator $\hat{\omega}$ by the relationship:

$$\underline{\Phi}(x,\lambda) = \phi(x,\lambda)/N(x) \qquad (1.30)$$

Section 1.4. The Eigenvalue Problem

The standard method of solving the transport equation (1.26) has been based on the assumption that by a separation of variables, a general solution can be expressed as a sum of terms of the form $\underline{\Phi}(x,\lambda)\exp(-\lambda t)$. A necessary and sufficient condition for the validity of this assumption is that the set of eigenfunctions be complete in a sufficiently general fuction space. In full the integro-operator eigenvalue problem becomes:

$$(A(x) - \lambda).\underline{\Phi}(x.\lambda) = \int dx' G(x|x').\underline{\Phi}(x',\lambda) \qquad (1.31)$$

where $A(x)$ is the so called 'Multiplicative Operator'.

There have been several investigations of the eigenvalue problem of the type (1.31) (see e.g. Shizuta 1964). The time behaviour of neutrons in matter as described by the linearised Boltzmann transport equation satisfies similar type of eigenvalue equation (Williams 1966). Some years ago it was realised by Case(1960) and others that the presence of $A(x)$ in (1.31) can introduce a 'continuum' eigenvalue spectrum, which must be used together with the discrete eigenvalues and the corresponding eigenfunctions to form a complete set. If we assume that $A(x)$ is a monotonically increasing function of x starting from its lowest value A_{min}, then for $\lambda \gg A_{min}$ there cannot be regular solutions of the equation because of the singularity at $A(x)=\lambda$.

However, it is still possible to find a continuum of solutions which turn out to be distributions in the sense of L.Schwartz (1966). For this reason, the equation is often called the 'singular eigenvalue' problem. The continuum spectrum arises through the use of a fundamental theorem of distribution theory which states that for any infinitely differentiable function $q(x)$ and for a simple zero x_o of $q(x)$, a distribution D_x satisfies the identity

$$q(x)D_x = 0 \qquad (1.32)$$

if and only if

$$D_x = C\delta(x-x_o) \qquad (1.33)$$

where C is a constant and $\delta(x-x_o)$ is the Dirac delta distribution. (The standard refrences on distribution theory are the monographs by L.Schwartz 1966, Lighthill 1958,

and Zemanian 1958).

More generally, the solution of equation

$$(x-x_0)g(x) = f(x) \qquad (1.34)$$

can be written as

$$g(x) = P.f(x)/(x-x_0) + \omega(x_0)\delta(x-x_0) \qquad (1.35)$$

The symbol P indicates that the principal value prescription must be used in any integral involving the integrand $f(x)/(x-x_0)$. $\omega(x_0)$ is an arbitrary function.

The first application of the above symbolic identity was made by* Van Kampen(1955) in a connection with a problem of plasma-oscillations and later by K.M.Case(1960), Mika(1961), Zelazny and Kuszell(1962) and others for solving one and two velocity dependent Boltzmann equation. By using (1.35) the formal solution of (1.31) for eigendistributions can be expressed as:

$$\underline{\Phi}(x,\lambda) = P.\int G(x|x')\underline{\Phi}(x',\lambda)dx' /(A(x)-\lambda) + \omega(\lambda)\delta(A(x)-\lambda) \qquad (1.36)$$

The formal solution above clearly indicates the singular nature of the eigenfunctions and the use of the terminology 'eigendistributions' for the eigenfunctions representing the continuum.

The problems of interpreting the right hand side of (1.36) were considered by Van Kampen in his original paper and more recently Hagelbroek (1973) has looked

* B. Davison (1944)

closely at the whole method of using eigendistributions. It is necessary to point out that Van Kampen and workers in neutron transport theory, including Hagelbroek, had to consider distributions of the form $f(x)/(x-x_0)$, where Cauchy principal value prescription followed quite naturally.

For more advaced type of singular eigenvalue problem (1.31) with $A(x)$ depending on the variable x in a complicated way, one would expect to find other types of distributions. Even for the 'Cauchy type' distributions, Hagelbroek has quite correctly pointed out all the difficulties associated with the application of the singular distributions from a rigorous mathematical point of view. Hagelbroek (1973) has attempted to resolve these difficulties by using the 'functional analytic' approach in order to make Case's method more clear and rigorous.

In chapter three, a unique set of eigendistributions is obtained which confirms the Case's method of solving the singular eigenvalue problem and at the same time gives a profound understanding of the whole topic.

In the absence of the singular eigenfunctions the initial value solution $h(x,t)$ can be expanded in terms of the discrete eigenfunctions $\underline{\Phi}(x,\lambda) = \underline{\Phi}_k(x)$. (where k now labels the discrete eigenvalues), provided that they form a complete set, in the following way:

$$h(x,t) = N(x) + \sum_k a_k \underline{\Phi}_k(x) \exp(-\lambda_k t) \qquad (1.37)$$

where the expansion coefficients are to be determined by the orthogonality property :

$$a_k = \int dx\, \underline{\Phi}_k(x) h(x,o) \qquad (1.38)$$

For discrete eigenfunctions the orthogonality property follows quite simply in a standard way, in the form:

$$\int dx \underline{\Phi}_n(x) . \underline{\Phi}_m(x) = 0 \qquad (1.39)$$

if $m \neq n$.

However, as was stated above and particularly in the neutron thermalisation problem by Koppel(1963) whenever A(x) is not independent of x, the discrete eigenfunctions must be supplemented by a continuum of singular solutions all orthogonal to the discrete set of eigenfunctions. Therefore, besides a linear combination of the discrete eigenfunctions, the general solution must contain a term given by an integral over the continuum:

$$h(x,t) = N(x) + \sum_K a_k \underline{\Phi}_k(x) \exp(-\lambda_k t) + \int_{\text{CONTINUUM}} d\lambda a(\lambda) \underline{\Phi}(x,\lambda) \exp(-\lambda t) \qquad (1.40)$$

Normally with the singular solutions the orthogonality condition is expressed as

$$\int dx\, \underline{\Phi}(x,\lambda') \underline{\Phi}(x,\lambda) = N(\lambda) \delta(\lambda - \lambda') \qquad (1.41)$$

where $N(\lambda)$, the normalisation function may be calculated by using the Poincare'-Bertrand formula (Koppel 1963):

$$P.\int 1/(\mu-\nu)\, d\mu\; P.\int 1/(\nu'-\mu)\, g(\mu,\nu')\, d\nu'$$

$$-\int d\nu' \int P.1/(\mu-\nu)\; P.1/(\nu'-\mu)\; g(\mu,\nu')d\mu = -\pi^2 g(\nu,\nu) \qquad (1.42)$$

(see e.g. K.M.Case and P.F.Zweifel 1967 page.70)
There are many unusual features associated with the application of (1.42) which are discussed in chapter three. Applying (1.41) to (1.40) we have

$$a(\lambda) = 1/N(\lambda) \cdot \int dx\, \Phi(x,\lambda)h(x,o) \qquad (1.43)$$

The Poincare'-Bertrand formula (1.42) works only for 'Cauchy principal value' distributions. In order to exchange the order of integration, in cases where the integrand contains other types of distributions, a Poincare'-Bertrand type of formula has to be found. For more information see the review article by Hoare (1971).

By using the theory of Laplace transforms, a tool recognised in the Linear transport theory literature to be the most powerful method of attacking initial value problems (see e.g. Corngold 1965), one can reduce the condition of validity of the eigenfunction expansion to the existence of a Laplace transform for any function $h(x,t)$. In chapter four, this method is applied and at the same time the connection with the singular eigenfunction method is established.

Section 1.5. The Model

The model we have considered was originally proposed by Rayleigh (1881). From the modern point of view, Rayleigh's original treatment was restricted to the study of an ensemble of very heavy test particles (or Rayleigh Pistons of mass M) undergoing brownian motion in a dilute gas (which serves as a heat-bath with particles of mass m). Rayleigh considered in detail the progress towards a stationary state and the nature of this state.

The modern extensions of the Rayleigh model have been concerned almost exclusively with the problem of Brownian motion. (see e.g. Green 1951, Akama and Siegel 1961). With the condition $M \gg m$ it is possible to reduce the initial value problem for $P(V,t)$ approximately to a second order partial differential equation. (the so called Rayleigh-Fokker-Planck equation). In chapter two, the model is reformulated in modern terminology and the validity of the R-F-Planck approximation is examined numerically. The numerical results are used to calculate the velocity autocorrelation function and hence using expressions from the linear response theory, the electrical conductivity of the model is obtained.

In chapter three, an exact solution is obtained by the singular eigenfunction method for the special Rayleigh model (essential where $m \neq M$). In chapter four, this model is solved by using the Laplace transform

method. A unique feature of this model is that 'absorbing barrier' problems can be formulated and solved exactly (chapter four). Although the general theory was developed exclusively for the spatially homogeneous transport equations, nevertheless, for the special Rayleigh model, the spatially dependent transport problem can be usefully studied (chapter five).

CHAPTER TWO

RAYLEIGH MODEL

Section 2.1. Preliminary Formulation

In order to introduce the Rayleigh model, one can do no better than quote from the original paper by Rayleigh in 1881:

" The investigations, of which a part is here presented, had their origin in a conviction that the present rather unsatisfactory position of the Theory of Gases is due in some degrees to a want of preparation in the mind of readers, who are confronted suddenly with ideas and processes of no ordinary difficulty. For myself, at any rate, I must confess that I have found great advantage from a more gradual method of attack, in which effort is concentrated upon one obstacle at a time. In order to bring out fundamental statistical questions, unencumbered with other difficulties, the motion is here limited to one dimension, and in addition one set of impinging bodies is here supposed to be very small relatively to the other. The simplification thus obtained in some directions allows interesting extensions to be made in others. Thus we shall be able to follow the whole process by which the steady state is attained, when heavy masses originally at rest are subjected to bombardment by projectiles fired upon them indifferently from both sides. ..... "

In modern terminology, the Rayleigh model can be described as an ensemble of test-particles of mass M, constrained to move in one dimension and bombarded by radom, impulsive collisions with a gas of heat-bath particles of mass m, having temperature T. One is interested in finding the evolution of the velocity probability distribution

P(V,t) satisfying the Master equation (1.16). As with most problems in physics, it is not always possible to find P(V,t) explicitly. Approximations and practical methods of solving the equation have been discussed by Hoare (1971).

In this chapter, the general problem for the test-particles of all possible mass-ratios,

$$\gamma = m / M \qquad (2.1)$$

free from restrictions imposed by Rayleigh (namely that $M \ggg m$) is discussed and a comparison is made with the limiting case of R-F-Planck equation. We begin by deriving the transition kernel for the model and later study the transport equation numerically.

Section 2.2. The Rayleigh Kernel

We consider the collision in one dimension of a piston of mass M with a particle of mass m. Let V, v be velocities before the collision and V', v' be the velocities after the collision. Applying the equation for conservation of energy and the equation for conservation of momentum, it follows that

$$M V^2 + m v^2 = M V'^2 + m v'^2 \qquad (2.2a)$$

and

$$M \underline{V} + m \underline{v} = M \underline{V}' + m \underline{v}' \qquad (2.2b)$$

From above it follows that

$$\underline{V}' = \frac{2\underline{v}.\gamma - \underline{V}.(\gamma-1)}{(1+\gamma)} \qquad (2.2c)$$

In order to calculate the Rayleigh transition kernel, we now suppose that the piston of mass M is immersed in a one dimensional heat-bath of point particles of mass m , kept at temperature T . One can consider any type of heat-bath but for this chapter it has been taken to be the Maxwellian distribution of velocities :

$$f_m(v) = (m/2\pi kT)^{\frac{1}{2}} \exp(-mv^2/2kT) \qquad (2.3a)$$

where k is the Boltzmann constant. It is convenient to write this in the form:

$$f_m(v) = C_o \exp(-\alpha v^2) \qquad (2.3b)$$

We require the probability $K(V|V')dV'$ that the piston having initial velocity $\underline{V}$ will go to a velocity in dV' about V' upon impulsive collisions. To obtain this let

$Z_+(v,V)$ = rate of collisions from left with V and v.
$Z_-(v,V)$ = rate of collisions from right with V and v.
or

$$Z(v,V) = C|V-v|f_m(v) \qquad (2.4)$$

where C is a frequency factor with dimensions $(\text{time})^{-1}.(\text{velocity})^{-1}$. To average over the outcome of all of all collisions, we use a method introduced

by Waldmann (1958) :

$$K(V|V') = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d\underline{v}d\underline{V}' \, \delta\left(V' - \frac{2\gamma\underline{v} + (1-\gamma)\underline{V}}{(1+\gamma)}\right) Z(v,V) \qquad (2.5)$$

The delta distribution in the above relationship expresses the conservation laws. By using the identity (see Zemanian 1958)

$$\int_a^b f(x)\delta(\alpha x-\beta)dx = 1/\alpha \; f(\beta/\alpha) \quad \alpha b > \beta > \alpha a$$
$$= 0 \qquad \text{otherwise} \qquad (2.6)$$

it can be shown that

$$K(V|V') = \mu \, Z(V'\mu + V(1-\mu),V) \qquad (2.7)$$

By using (2.4) and (2.3) the above relationship can be expressed as

$$K(V|V') = \mu^2 C_0 |V-V'| \exp(-\alpha[(V'-V).\mu + V]^2) \qquad (2.8)$$

where

$$\mu = (1+\gamma)/2\gamma$$

The above kernel was not derived by Rayleigh but was explicitly given by Lebowitz and Bergmann (1957). The Master equation for the Rayleigh model can be written as

$$\frac{\partial P(V,t)}{\partial t} = \int_{-\infty}^{\infty} dV' K(V'|V)P(V,t) - Z(V)P(V,t) \qquad (2.9)$$

where Z(V) is the velocity dependent collision number given by

$$Z(V) = \int_{-\infty}^{\infty} dV' K(V \mid V')$$

$$= C\,V.\ \mathrm{erf}\left((m/2kT)^{\frac{1}{2}} V \right) + (2kT/\pi m)^{\frac{1}{2}} \exp(-mV^2/2kT).C \qquad (2.10)$$

which can be derived by a straightforward integration by parts. The Maxwellian distribution for the ensemble is

$$f_M(V) = (M/2\pi kT)^{\frac{1}{2}} \exp(-MV^2/2kT) \qquad (2.11)$$

from which by direct calculation we see that the kernel satisfies the detailed balance condition

$$f_M(V)K(V|V') = f_M(V')K(V'|V) \qquad (2.12)$$

which immediately implies that the Maxwellian distribution is the equilibrium distribution for the ensemble. The conservation of probability condition is

$$\int_{-\infty}^{\infty} dV P(V,t) = 1 \qquad (2.13)$$

In order to make further analysis simple, one can introduce the following reduced variables:

$$\begin{aligned} x &= (m/2kT)^{1/2} \cdot V \\ y &= (m/2kT)^{1/2} \cdot V' \\ \tau &= (2kT/\pi m)^{1/2} \cdot C.t \end{aligned} \qquad (2.14)$$

By defining

$$P(x,\tau) = (2kT/m)^{\frac{1}{2}} P\left((2kT/m)^{\frac{1}{2}}x, (\pi m/2kT)^{\frac{1}{2}}\tau/C \right) \qquad (2.15)$$

the transport equation can be written in the form:

$$\frac{\partial P(x,\tau)}{\partial \tau} = \mu^2 \int_{-\infty}^{\infty} dy\,|x-y| \exp(-[(x-y)\mu+y]^2) P(y,\tau) - z(x)P(x,\tau) \qquad (2.16)$$

where the kernel and the collision number in reduced variables are

$$k(x|y) = \mu^2 |x-y| \exp(-[(y-x)\mu+x]^2) \qquad (2.17)$$

$$z(x) = \int_{-\infty}^{\infty} dy\, k(x|y)$$

$$= \exp(-x^2) + \pi^{\frac{1}{2}} x \operatorname{erf}(x) \qquad (2.18)$$

where the error function is defined by the integral

$$\operatorname{erf}(x) = 2/\pi^{\frac{1}{2}} \int_0^x du \exp(-u^2) \qquad (2.19)$$

the equilibrium distribution in the reduced variables becomes

$$f_M(x) = (2kT/m)^{\frac{1}{2}} f_M\left((2kT/m)^{\frac{1}{2}} x \right)$$

$$= \exp(-x^2/\gamma)/(\pi\gamma)^{\frac{1}{2}} \qquad (2.20)$$

It is useful to list all the properties of the collision number which will be required later. (Hoare and Rahman 1973/74).

Figure 1.

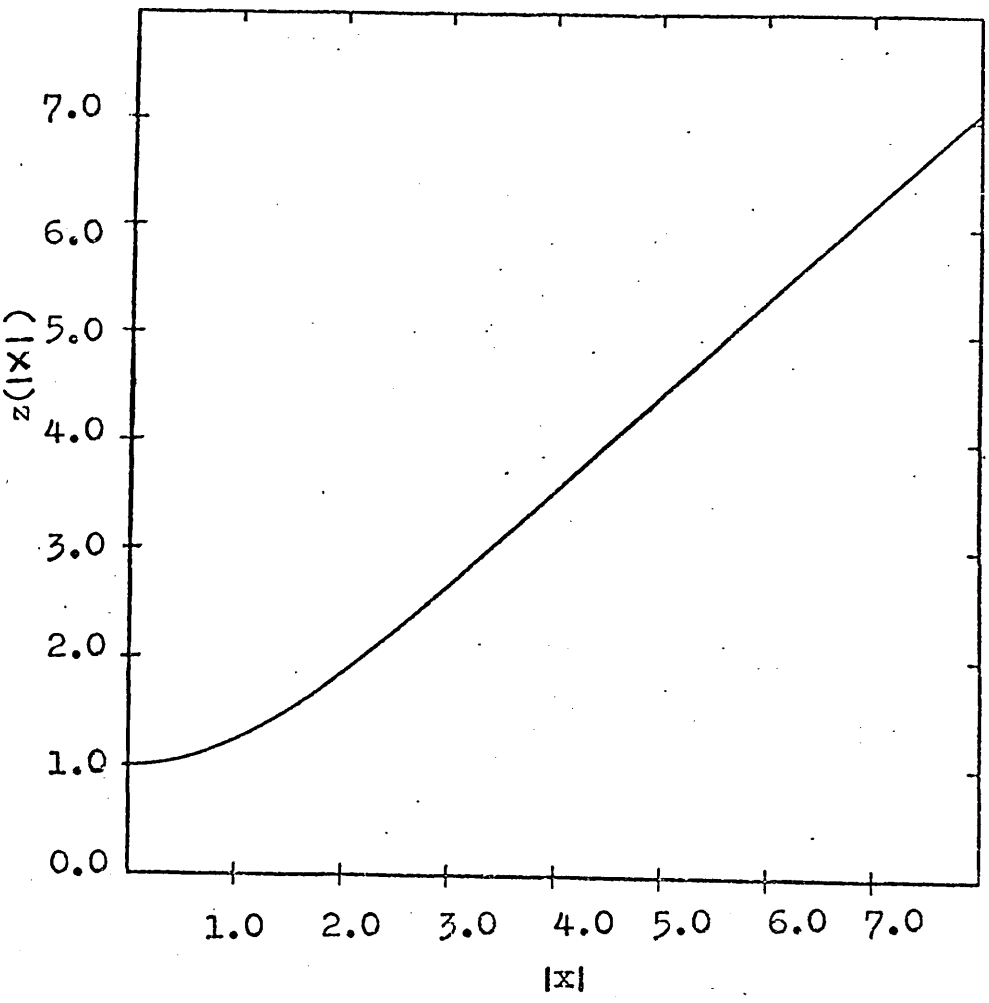


Figure Caption

The collision-number function $z(|x|)$ for Rayleigh pistons in terms of reduced variable x. The velocity collision-number curve is the same with symmetric reflection about the y axis.

(i) $z(x)$ is a single valued and analytic function for all x in the range $(-\infty,\infty)$.

(ii) $z(x)$ is an even function: $z(x) = -z(-x)$.

(iii) for large $|x|$, $z(x) \sim |x|\pi^{\frac{1}{2}}$. (2.21)

(iv) $z(x)$ is a monotonically increasing function from its minimum value at $z(o) = 1$. (see Figure 1.)

(v) for small x, $z(x) \sim 1 + x^2 + O(x^4)$ (2.22)

(vi) $z(x)$ is infinitely differentiable with

$$z'(x) = \pi^{\frac{1}{2}}\mathrm{erf}(x) \qquad (2.23)$$

$$z''(x) = 2\exp(-x^2) \qquad (2.24)$$

and $z(x)$ satisfies the differential equation:

$$z''(x) + 2xz'(x) - 2z(x) = 0. \qquad (2.25)$$

Section 2.3. Eigenvalue Spectrum and the R-F-Planck equation

From chapter one (1.23) it follows that the eigenvalue problem for the transport equation (2.16) can be written as

$$(z(x) - \lambda)\phi(x,\lambda) = \mu^2\int_{-\infty}^{\infty} dy\,|x-y|\exp(-[(x-y).\mu + y]^2)\,\phi(y,\lambda) \qquad (2.26)$$

and the corresponding symmetrised equation (1.31) follows as

$$(z(x) - \lambda).\underline{\phi}(x,\lambda) = \int_{-\infty}^{\infty} dy\,g(x|y).\,\underline{\phi}(y,\lambda) \qquad (2.27)$$

where

$$g(x|y) = \mu^2 |x-y| \exp(-[x^2 + y^2]/2).\exp(- \mu(\mu-1).(x-y)^2) \qquad (2.28)$$

$$\bar{\Phi}(x,\lambda) = \phi(x,\lambda)/N(x) \qquad (2.29)$$

$$N(x) = \exp(-x^2/2\gamma)/ (\pi\gamma)^{1/4} \qquad (2.30)$$

Hoare and Rahman (1973/74) have examined the general properties of the eigenfunction equation (2.27). The equlibrium eigenvalue $\lambda=0$ is always present for all values μ ($\infty > \mu > \frac{1}{2}$), corresponding to the equilibrium distribution. In general, the continuum part of the spectrum extends from $z(o) = 1$ along the entire positive axis to infinity. The discretum always contains the eigenvalue $\lambda=0$ and in general; may either be empty, or contain a finite number of eigenvalues, or an infinite number necessarily with a point of accumulation. It is possible that discrete eigenvalues can exist in the continuum region but for physical systems this is a remote possibility.

Hoare and Rahman (1973/74) have shown that the non-zero eigenvalues are bounded for a finite mass ratio γ being in fact completely absent for the special Rayleigh model or $\gamma = 1$. A tentative bound was obtained which suggested that the discretum must be empty (except for $\lambda=0$ eigenvalue) at least for the mass-ratio region:

$$\{3(2^{\frac{1}{2}} - 1)\}^{-1} \leqslant \gamma \leqslant 3(2^{\frac{1}{2}} - 1)$$

In the next section a numerical study of the eigenvalue problem is presented and the validity of the tentative bound is tested.

In Rayleigh's original paper and subsequently attention has been directed not at the eigenvalue equation (2.27) but on the related R-F-Planck equation and its counterpart the Langevin equation (Chandrasekhar 1943). Since the Master equation can only be solved in rare cases, it is important to know, under what circumstances the F-Planck equation is a good approximation. Razavy (1976) has looked at the approach to Brownian motion in case of a solvable kernel where the continuum is missing because of the nature of the simplified kernel and has confirmed the weakness of the approximation.

The Master equation (2.16) can be expressesd in terms of the Krammer-Moyal expansion series (Sigel 1960) as

$$\frac{\partial P(x,\tau)}{\partial \tau} = \sum_{n=1} \frac{1}{n!} \left(-\frac{\partial}{\partial x}\right)^n a_n(x).\ P(x,\tau) \qquad (\ 2.31\ )$$

in terms of the 'derivate moments' $a_n(x)$ (using Moyal's terminology; Moyal 1949)

$$a_n(x) = \int_{-\infty}^{\infty} dy (y-x)^n k(x|y) \qquad (\ 2.32\ )$$

By expanding the first two moments in the lowest powers of γ and retaining only the first two moments in (2.31) the

R-F-Planck equation

$$\frac{1}{4\gamma}\frac{\partial P(x,\tau)}{\partial \tau} = \frac{\partial}{\partial x}\,x\,P(x,\tau) + \frac{\gamma}{2}\frac{\partial^2 P(x,\tau)}{\partial x^2} \qquad (2.33)$$

can be derived in terms of the reduced variables. (see e.g. Hoare and Rahman 1973/74). This equation suggests a new time scale $\tau_R = 4\gamma\tau$. The differential operator appearing on the right-hand side of (2.33) is called the Rayleigh operator

$$\hat{\omega}_R = \frac{\partial}{\partial x}\,x + \frac{\gamma\,\partial^2}{2\,\partial x^2}$$

Hence we can write

$$\frac{\partial P(x,\tau_R)}{\partial \tau_R} = \hat{\omega}_R P(x,\tau_R) \qquad (2.34)$$

The corresponding eigenvalue equation is

$$\hat{\omega}_R \phi_n(x) = -\lambda_R \phi_n(x) \qquad (2.35)$$

with

$$\phi_n(x) = \exp(-x^2/2\gamma)\cdot H_n(x/\gamma^{\frac{1}{2}})\frac{1}{(2^n n!\,\pi\gamma)^{\frac{1}{2}}} \qquad (2.36)$$

and

$$\lambda = 0,1,2,3,4,\ldots\ldots$$

$H_n(x)$ is the n^{th} order Hermite polynomial. For the special initial condition $P(x,o) = \delta(x-x_o)$, using Mehler's formula (Erdelyi 1953), the solution follows as

$$P(x,\tau_R) = \exp(-x^2/\gamma)\cdot\sum_n (2^n n!\pi\gamma)^{-1} H_n(x/\gamma^{\frac{1}{2}}) H_n(x_o/\gamma^{\frac{1}{2}}) \exp(-n\tau_R)$$

$$= \exp\left\{ \frac{-(x-x_o\cdot\exp(-\tau_R))^2}{\Delta(\tau_R)\cdot\gamma} \right\} \rho \cdot \frac{1}{\Delta(\tau_R)^{\frac{1}{2}}}$$

(2.37)

where

$$\Delta(\tau_R) = 1 - \exp(-2\tau_R)$$

We see that in τ_R-time scale, the R-F-Planck approximation for small γ, consists of discrete lines and the continuum region, from $\lambda = 1$ to infinity, is approximated by the discrete eigenvalues with $n > 1/4\gamma$. It must be pointed out that in real time scale t, the continuum would always be present. The approximate solution even for quite small mass-ratio γ must falsify behaviour for small time because then the continuum would determine the rate of relaxation. It is quite difficult to make qualitative statements about the validity of the approximation. For example, numerically how small γ must be before the equation describes adequately over some time range the evolution of the test-particle ensemble.

The numerical results obtained in the next section have been used to test the discrepancy between the discrete eigenvalues and the integer-eigenvalues λ_R of equation (2.35). A similar study was carried out by Hoare and Kaplinsky (1970/75) for the three dimensional hard sphere gas.

Section 2.4. Numerical Study

Of all avaliable practical methods of finding the eigenvectors and eigenvalues of the Master equation (2.16), the simplest is perhaps the method of discretisation. One can use the Rayleigh-Ritz method (Hoare and Kaplinsky 1970/75) or one of the other methods described in detail by Hoare (1971). But the numerical method of discretisation is probably equally efficient and can be used without too much labour and computation. In any case, the direct method of discretising the eigenvalue problem can be used to give preliminary information about the spectrum, even if later, more appropriate methods are to be applied.

The symmetrised eigenvalue equation (2.27) is discretised in order to obtain results not tied to any particular initial distribution. This way of solving transport equation is quite common in neutron transport theory and the monographs by Williams contains many examples.(Williams 1966/71). Wood (1965) has used the method to obtain numerical results for the hard sphere gas.

Working in the symmetric form of the eigenvalue problem (2.26) we arrive at the following matrix eigenvalue equation:

$$(\tilde{z}_i - \lambda)\,\tilde{\Phi}_i(\lambda) = \sum_{j=1}^{N} \tilde{g}_{ij}\,\tilde{\Phi}_j(\lambda) \qquad (2.38)$$

where we have used tilde for the discretised approximations

In matrix notation this eigenvalue equation reads:

$$(\tilde{\tilde{Z}} - \lambda\tilde{\tilde{I}}) \circ \underline{\tilde{\Phi}} = \tilde{\tilde{G}} \circ \underline{\tilde{\Phi}} \qquad (2.39)$$

To make this approximation self consistent the vector $\tilde{Z}$ is calculated numerically by using the relationship (1.24)

$$z(x) = \int_{-\infty}^{\infty} dy\, g(x|y) \circ \frac{N(y)}{N(x)} \qquad (2.40)$$

Therefore,

$$\tilde{Z}_i = h\exp(+(ih)^2/2\gamma) \sum_{j=i}^{N} G(ih,jh).\exp(-(jh)^2/2\gamma) \qquad (2.41)$$

where h is the size of the mesh interval, N the number of intervals and G(ih,jh) the matrix elements of the matrix G. With this way of calculating the matrix $\tilde{Z}$, the eigenvalue $\lambda = 0$ always corresponds to the equilibrium-vector or the equilibrium distribution. The converged numerical eigenvalues $\lambda_k < 1$ are good estimates of the discrete eigenvalues and the numerical eigenvalues $\lambda_k > 1$ (we shall refer to these as pseudo-eigenvalues) represent "approximately" the continuum region. It is not clear how the pseudo-eigenvalues converge with increasing N and fixed range R, to exihibit the continuum contribution (h = 2R/N). If the discretum is empty except for the eigenvalue $\lambda = 0$ then it is clear that any calculation of physical properties must involve summation over the pseudo-eigenvalues.

Perhaps when discretising a singular eigenvalue

problem one ought to regard the whole set of discrete eigenvalues as representing the spectrum. If one adopts this approach then the numerical eigenvalues and eigenfunctions can be used to solve the initial value problem at least over a specified time range. It will most certainly falsify the evolution of the system for small times. By increasing the range and decreasing the mesh interval h, one would expect the numerically constructed solutions to give improved description of the relaxation process.

A special feature of the numerical method is that one can study the first few eigenvalues by choosing a small range R and taking a large number of intervals. For studying the time dependent distribution $P(x,\tau)$, a large number of eigenvalues have to be considered. Thus $\tilde{\lambda}_k$ may not be a good approximation to some particular <u>true</u> eigenvalue but nevertheless the whole set of numerical eigenvalues $\tilde{\lambda}_k$ may serve sufficiently to represent the evolution of the distribution. Thus, in case of physically interesting functions, such as the average velocity function for the ensemble or the autocorrelation function, it may be quite futile to search for the <u>true</u> eigenvalues and eigenfunctions. It is very difficult to quantify these concepts and to develop a meaningful method of estimating the errors involved. (A mean square criterion for the Rayleigh-Ritz method was developed by Hoare and Kaplinsky 1975).

There are many problems in physics where the continuum contribution plays a very important part and should not be neglected. In the study of two electron-atoms,

Burke (1976) has emphasised this point:

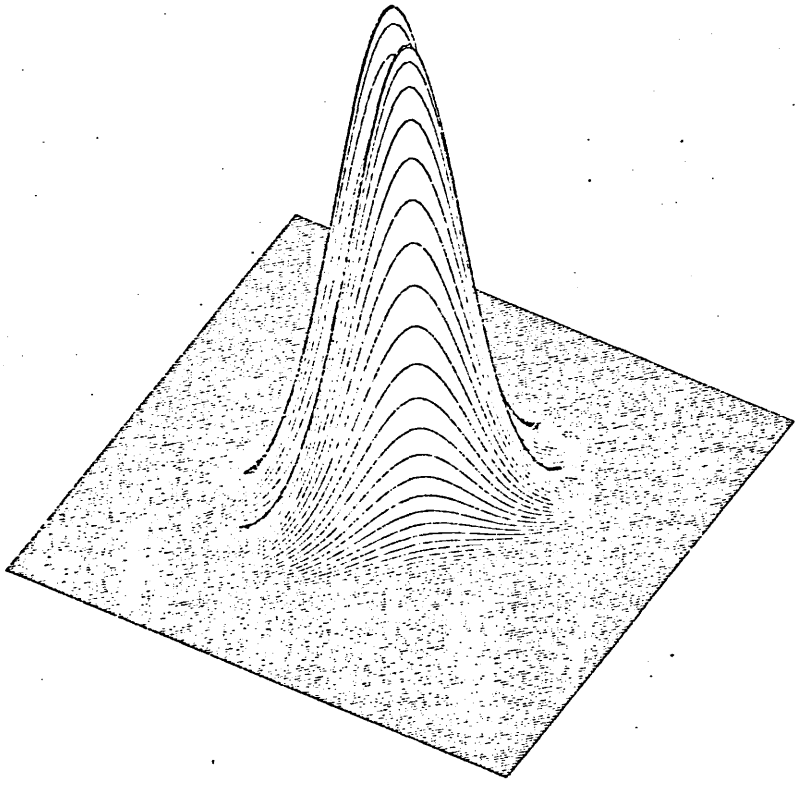
" Unfortunately experience has shown that this expression (in terms of a few atomic eigenstates) is slowly convergent at intermediate energies and indeed important contributions arise from the continuum eigenstates which cannot easily be included. One proposal to overcome this difficulty is to include a few well chosen pseudo-states which are not target eigenstates. The results indicate that with sufficient efforts perhaps 10-20 % accuracy can be obtained at intermediate energies using this pseudo-state method, but other non-physical effects such as the pseudoresonances and pseudothresholds preclude the attainment of higher accuracy at the moment. This statement is also relevant to electron scattering by complex atoms and ions with more than one electron. "

For the special Rayleigh model the discretum contains only the equilibrium eigenvalue $\lambda = 0$. (see chapter three and Hoare and Rahman (1973/74)). In a later chapter, the exact expression for the velocity autocorrelation function $S_x(\tau)$ is obtained for the special model. We were able to test the 'pseudo-eigenstate' approximation by calculating from numerical eigenvalues for $\gamma = 1$ $S_x(\tau)$ and comparing the result with the exact solution. To within about 10-15 % the results agree and as expected the agreement is worse for small times. This detailed study may also be of some interest to physicists working in Quantum theory and elsewhere where the continuum plays a very important part.

Section 2.5. Numerical Analysis

In order to aproach the 'accurate numerical' eigenvalues we used the drawing in three dimension of the symmetric

Figure 2



The kernel $G(x|y)$ for mass ratio $\gamma = 0.5$. The vertical scale is arbitrary, the x and y intervals plotted run from -10 to +10 with the origin at centre of the diagram. Note the symmetric nature of the kernel.

kernel $g(x|y)$. Using these diagrams, the actual range is choosen such that the values of the kernel outside the range are too small to be of computer significance (using 'single precision' CDC arithatic). Next the eigenvalues and eigenvectors of interest are computed by using a small number of mesh points ($N \sim 50$) and the range. From this initial study it is possible to find the smallest possible value of the range such that all eigenvectors corresponding to eigenvalues of interest are 'non-zero' only outside this range. Finally by using this range and a large number of intervals, the eigenvectors and eigenvalues are computed. It was possible to use up to 400 intervals.

The eigenvalue subroutines were from the NAG Library and all computations were performed on the University of London Computer Centre (U.L.C.C.) CDC 7600 machine. The U.L.C.C. 'SYMVU' package was used to produce the drawings of the symmetric kernel. The special case $\gamma = 1$ was used throughout as a test case to check the routines and the numerical results.

Section 2.6. Results and Interpretations

(a) Approach to Brownian motion and Eigenvalue Spectrum

In order to make the comparision between the numerical eigenfunctions and the R-F-Planck solutions (2.35) $\phi_n(x)$, the latter set of functions have been used as a basis to expand the eigenfunctions $\tilde{\phi}_k(x)$ and look for the ' impurity ' present in each Fourier-Hermite component. Tables are

Caption For Tables I to VI

Rayleigh-Eigenfunctions in the Hermite representation.

Each column gives the expansion coefficients for the eigenfunction $\tilde{\phi}_k(x)$ with respect to the set $\phi_n(x)$.

The dashes indicate values absorbed into the continuum.

Gamma = 2^{-2}

λ_R = 0.00000	0.89239	-	-	-	-	-	-	-	
k i= 0	1								
0 1.00000	.00000	-	-	-	-	-	-	-	
1 0.00000	.99562	-	-	-	-	-	-	-	
2 0.00000	.00000	-	-	-	-	-	-	-	
3 0.00000	-.08959	-	-	-	-	-	-	-	
4 0.00000	.00001	-	-	-	-	-	-	-	
5 0.00000	.02397	-	-	-	-	-	-	-	
6 -.00002	.00014	-	-	-	-	-	-	-	
7 0.00000	-.00988	-	-	-	-	-	-	-	
8 -.00004	.00030	-	-	-	-	-	-	-	

Gamma = 2^{-3}

λ_R =	0.00000	0.94139	1.66442	-	-	-	-	-	-
k	i= 0	1	2						
0	0.99999	.00000	.00000	-	-	-	-	-	-
1	0.00000	.99944	.00000	-	-	-	-	-	-
2	0.00000	.00000	.99399	-	-	-	-	-	-
3	0.00001	-.03310	.00001	-	-	-	-	-	-
4	0.00002	.00000	-.10748	-	-	-	-	-	-
5	0.00000	.00346	.00030	-	-	-	-	-	-
6	-.00001	-.00062	.00002	-	-	-	-	-	-
7	0.00000	.00007	.00003	-	-	-	-	-	-
8	0.00000	.00008	-.00548	-	-	-	-	-	-

Gamma = 2^{-4}

λ_R=	0.00000	0.96982	1.82346	2.57328	3.22952	3.22952	-	-	-
k	i= 0	1	2	3	4	5			
0	0.99999	.00000	.00000	.00000	.00000	.00000	-	-	-
1	0.00000	.99989	.00000	.01448	.00000	.00063	-	-	-
2	0.00000	.00000	.99903	.00000	.04370	.00000	-	-	-
3	-.00001	-.01449	.00001	.99568	.00000	.09004	-	-	-
4	0.00000	.00000	-.04381	.00009	.98586	.00004	-	-	-
5	0.00000	.00063	.00004	-.09083	.00044	.96149	-	-	-
6	0.00006	.00002	.00307	.00022	-.15915	.00157	-	-	-
7	0.00000	-.00021	.00012	.00925	.00077	-.25255	-	-	-
8	0.00000	.00005	-.00120	.00045	.02209	.00187	-	-	-

Gamma = 2^{-5}

λ_R=	0.00000	0.94632	1.83613	2.76440	3.46240	4.39497	4.90453	6.16978	6.87916
k	i= 0	1	2	3	4	5	6	7	8
0	0.99999	.00000	.00000	.00000	.00003	.00002	.00000	.00001	.00000
1	0.00000	.99999	.00000	.00000	.00001	.00000	.00000	.00000	.00003
2	0.00001	.00000	.99984	.00000	.01896	.00000	-.00056	.00001	.00000
3	0.00002	-.00650	.00000	.99930	.00000	.03785	.00000	.00178	.00000
4	-.00003	.00000	-.01896	.00000	.99777	.00000	.06368	.00007	.00006
5	0.00000	.00013	.00001	-.03786	-.00001	.99457	.00000	-.09632	.00000
6	0.00000	.00000	.00064	.00000	-.06375	.00010	.98791	-.13789	-.00025
7	0.00000	.00000	.00000	.00187	-.00004	-.09736	.00004	.97564	-.00001
8	-.00001	.00000	-.00005	.00002	.00426	.00020	-.13989	.00165	.95335

Gamma = 2^{-6}

λ_R= 0.00000	0.99245	1.95424	2.88640	3.79048	4.67028	5.53489	6.40040	7.28600
k i= 0	1	2	3	4	5	6	7	8
0 0.99999	.00000	.00011	.00000	.00000	.00000	.00000	.00000	.00000
1 0.00000	.99999	.00000	-.00348	.00000	-.00002	.00000	-.00001	.00000
2 0.00030	.00000	.99998	.00000	.00974	.00000	.00015	.00000	.00003
3 0.00000	-.00349	.00000	.99995	.00006	.01915	.00008	.00060	.00003
4 0.00000	.00000	.00985	-.00016	.99987	.00037	.03258	.00039	.00248
5 0.00000	-.00002	.00006	.01993	.00092	.99970	.00151	.05221	.00124
6 -.00001	.00003	-.00029	-.00035	-.03561	-.00374	.99937	-.00409	.08128
7 0.00000	-.00018	.00016	.00203	.00142	.06736	.01087	.99882	.00757
8 0.00004	.00005	-.00110	-.00103	.00067	-.00876	.00359	-.12663	.99797

Gamma = 2^{-7}

λ_R= 0.00000	0.99744	1.99739	2.94607	3.89775	4.83484	5.75852	6.67232	7.58478
i= 0	1	2	3	4	5	6	7	8
k								
0 1.00000	.00000	.00011	.00000	.00000	.00000	.00000	.00000	.00000
1 0.00000	.99999	.00000	.00141	.00000	.00001	.00000	.00000	.00000
2 0.00011	.00000	.99999	.00000	.00431	.00000	.00000	.00002	.00000
3 0.00000	.00141	.00000	.99996	.00000	.00861	.00000	.00009	.00000
4 0.00000	.00000	.00432	.00000	.99987	.00002	.01438	.00003	.00002
5 0.00000	.00000	.00001	.00002	.00863	.99962	.00015	.02015	.00019
6 0.00000	.00000	.00002	.00001	.01457	.00030	.99882	.00069	.03220
7 0.00000	.00000	.00000	.00001	.00011	.00139	.02285	.99629	.00233
8 0.00001	.00000	.00005	.00044	.00053	.03618	.00479	.00510	.98876

Figure 3

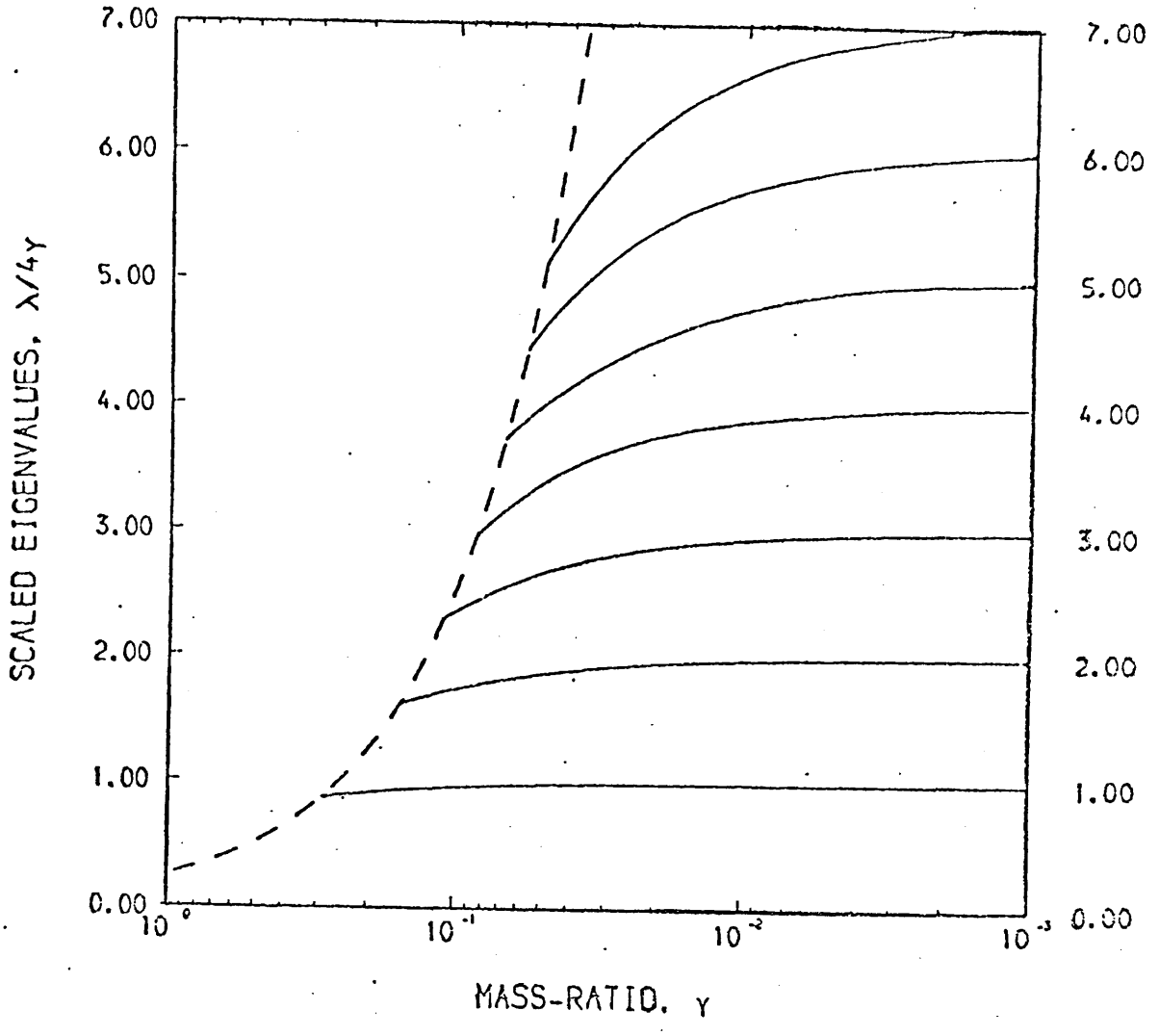


Figure Caption

Converged Numerical Eigenvalues of the Rayleigh Kernel as a function of mass ratio γ. The time is scaled according to (2.34) and in this units the continuum is the region within the dashed curve. On the right the eigenvalues are seen approaching the integer values predicted by the Fokker-Planck equation, the effectiveness of this approximation decreasing progressively with higher indices.

Figure 4

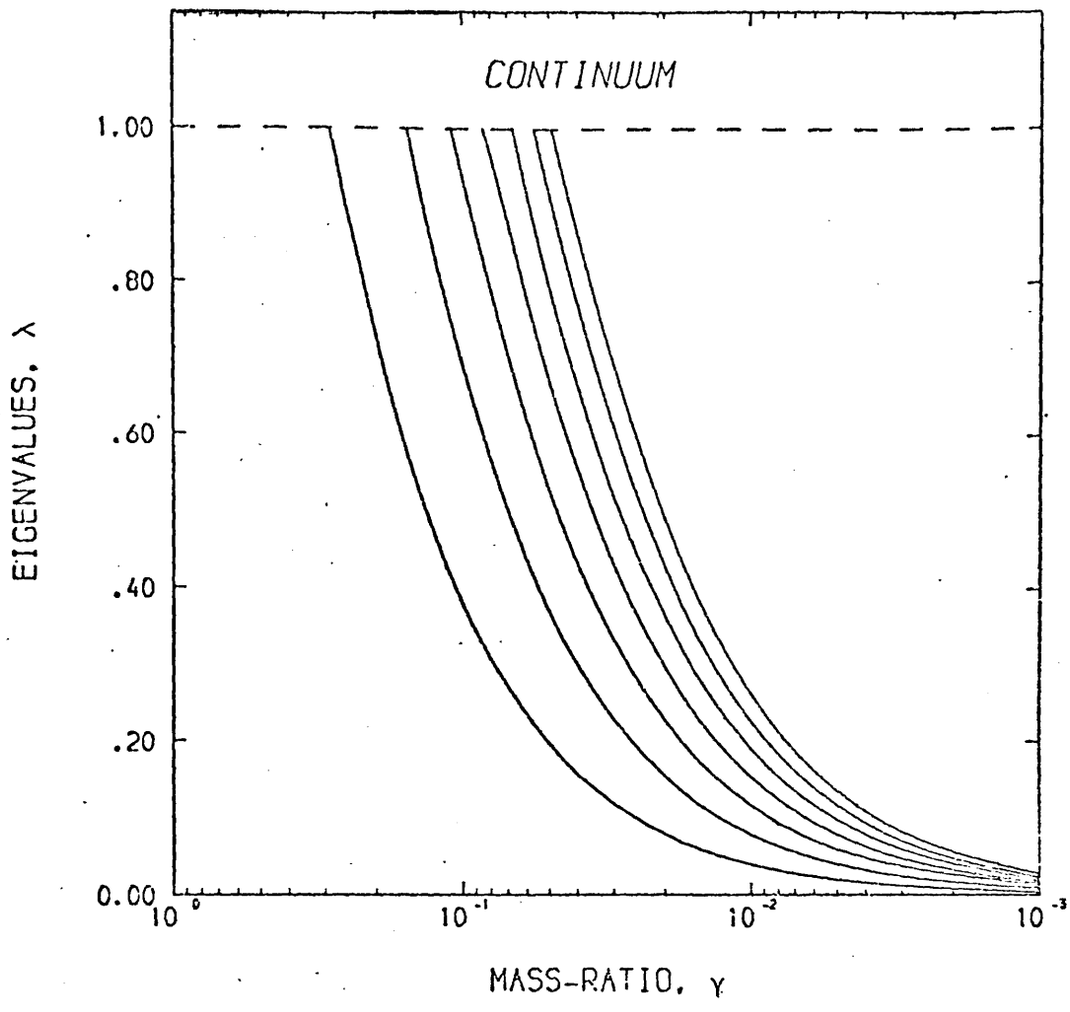


Figure Caption

Numerical Eigenvalues of the Rayleigh Kernel as a function of mass ratio γ. The discretum is seen to be empty in the region $0.28 < \gamma < \infty$.

presented of these results for various values of the mass ratio γ.

The approach to Brownian motion behaviour with decrease in the mass ratio γ exhibits itself with progressive convergence of an increasing number of true eigenfunctions to the corresponding Fokker-Hermite basis set functions $\phi_n(x)$. At the same time, begining with the first few eigenvalues , the discrete spectrum (Figure 3) steadily converges to the corresponding Fokker-Planck spectrum. As expected χ_k in τ_R-time scale do approach integral values for sufficiently small mass ratios, however, it is impossible to make quantitative statements about the R-F-Planck approximation from the numerical results. One can say with with some certainty that after a long time the relaxation of the system would be dominated by the first few discrete eigenvalues and therefore the R-F-Planck approximation will be good for mass-ratios of value less than about 10^{-3} and for aged systems.

We note from Figure 4 that the emptiness of the discretum actually extends over the mass ratio region $0.28 < \gamma < \infty$.

(b) Velocity Autocorrelation Function $S_x(\tau)$

Instead of the correct initial solution (1.37) we arrive at the approximate solution

$$h(x,\tau) = \tilde{N}(x) + \sum_K a_k \tilde{\phi}_k(x) \exp(-\hat{\lambda}_k \tau) \qquad (2.42)$$

with the approximate eigenvalues $\hat{\lambda}_k$ and the eigenvectors $\tilde{\Phi}_k(x)$. In the above summation we have included all the pseudo-eigenstates. In order to obtain the physically interesting velocity autocorrelation function (in the original variables)

$$S_V(t) = \langle \rho(o).\rho(t) \rangle_{eq.} \qquad (2.43)$$

where $\rho(t) = \langle V(t) \rangle - \langle V(oo) \rangle$

(the second average is over the equilibrium ensemble) we have to consider the fundamental initial condition $P(V,O) = \delta(V-V_o)$. Thus

$$\rho(o) = V_o \quad \text{and} \quad \rho(t) = V(t)$$

Therefore,

$$S_V(t) = \int_{-\infty}^{\infty} dV_o V_o f_M(V_o) \int_{-\infty}^{\infty} dV\ V\ P(V,t;V_o) \qquad (2.44)$$

In terms of the reduced variables x and τ, equation (2.44) can be expressed in the form

$$S_V(t) = \int_{-\infty}^{\infty} \frac{dx_o x_o \exp(-x_o^2/\gamma)}{\gamma^{\frac{1}{2}}} \int_{-\infty}^{\infty} dx\ x/\gamma^{\frac{1}{2}}\ P(x,\tau) \left(\frac{2kT}{M\pi}\right)^{\frac{1}{2}}$$

$$= (2kT/\pi M)^{\frac{1}{2}} S_x(\tau) \qquad (2.45)$$

But from (2.42) for the initial condition $P(x,o)=\delta(x-x_o)$ we arrive at the approximate solution:

$$h(x,\tau) = \tilde{N}(x) + \sum_{k} \tilde{\Phi}_k(x_o)\, \tilde{\Phi}_k(x) \frac{\tilde{N}(x)}{\tilde{N}(x_o)} . \exp(-\hat{\lambda}_k \tau) \qquad (2.46)$$

Therefore,

$$\langle x(\tau)/\gamma^{\frac{1}{2}} \rangle = \sum_{k} \frac{\tilde{\Phi}_k(x_o)\; E_{ok} . \exp(-\hat{\lambda}_k \tau)}{\tilde{N}(x_o)} \qquad (2.47)$$

where

$$E_{ok} = \int_{-\infty}^{\infty} dx\; (x/\gamma^{\frac{1}{2}}) .\; \tilde{N}(x) .\; \tilde{\Phi}_k(x) \qquad (2.48)$$

But the eigenvectors $\tilde{\Phi}_k(x)$ can be expanded in terms of the Fokker-Hermite functions $\phi_n(x)$:

$$\tilde{\Phi}_k(x) = \sum_{j} \alpha_j \phi_j(x) \qquad (2.49)$$

with

$$\tilde{N}(x) = \phi_o(x) .$$

By substituting in (2.48) it follows that

$$E_{ok} = \int_{-\infty}^{\infty} dx \sum_{j} \alpha_j \phi_o(x) . (x/\gamma^{\frac{1}{2}}) .\; \phi_j(x)$$

$$= \sum_{j} \alpha_j \cdot \langle o \,|\, (x/\gamma^{\frac{1}{2}}) \,|\, j \rangle \qquad (2.50)$$

in Dirac quantum mechanical notation. Using the property (see e.g. Schieff 1955)

$$\langle o|(x/\gamma^{\frac{1}{2}})|\, j \rangle = (1/2)^{\frac{1}{2}} \delta_{o,j-1} + \delta_{o,j+1} \qquad (2.51)$$

it follows that

$$E_{ok} = (1/2)^{\frac{1}{2}} . \alpha_1 \qquad (2.52)$$

Therefore,

$$\langle x(\tau)/\gamma \rangle = \sum_K \frac{(1/2)^{\frac{1}{2}} \alpha_1 \tilde{\Phi}_k(x_o) \exp(-\hat{\lambda}_k \tau)}{\tilde{N}(x_o)} \qquad (2.53)$$

and

$$S_x(\tau) = \sum_K e^{-\lambda_k \tau} . (\alpha_1 / 2^{\frac{1}{2}}) \int_{-\infty}^{\infty} dx_o \tilde{N}(x_o) x_o \tilde{\Phi}_k(x)$$

$$= \sum_K (\alpha_1^2/2) . \exp(-\hat{\lambda}_k \tau) \qquad (2.54)$$

by expanding $\Phi_k(x)$ as in (2.49) above etc.

(c) Electrical Conductivity in Linear Response Regime

To the approximations of the linear response theory (Kubo 1957) it can be shown that the admittance σ of an ensemble of Rayleigh test-particles of charge e is given by

$$\sigma = \sigma_o \int_o^{\infty} d\tau \exp(i\omega\tau)\, S_x(\tau) \qquad (2.55)$$

In the above expression σ_o is a suitable constant. Using (2.54) the above expression becomes

$$(\sigma / \sigma_o) = \sum_K (\alpha_1^2 / 2) \frac{1}{(\lambda_k - i\omega)}$$

$$= \sum_K \frac{\alpha_1^2 . (\lambda_k + i\omega)}{(\lambda_k^2 + \omega^2)} \qquad (2.56)$$

(d) Numerical Computations

It will suffice here to present a small selection of results designed to illustrate the main characteristics of the auto-correlation function (for different values of mass ratio γ.) and the electrical conductivity.

Autocorrelation Function

Figure 5 shows the full velocity autocorrelation function $S_x(\tau)$ for equlibrium fluctuations according to (2.54). Mass ratio γ takes the values 2^0, 2^{-1}, 2^{-2}, 2^{-3}, 2^{-4}, 2^{-5}, 2^{-6} and 2^{-7}. The relaxation process slows down as the mass ratio decreases because the discretum eigenvalues begin to dominate. The autocorrelation function for mass ratio 2^{-2} and 2^{-3} is nearly the same as one would expect from the presence of effectively one discrete eigenvalue. The autocorrelation function for 2^{-7} is nearly identical to the result one would obtain if the process was described by the Rayleigh-Fokker Planck approximation i.e.

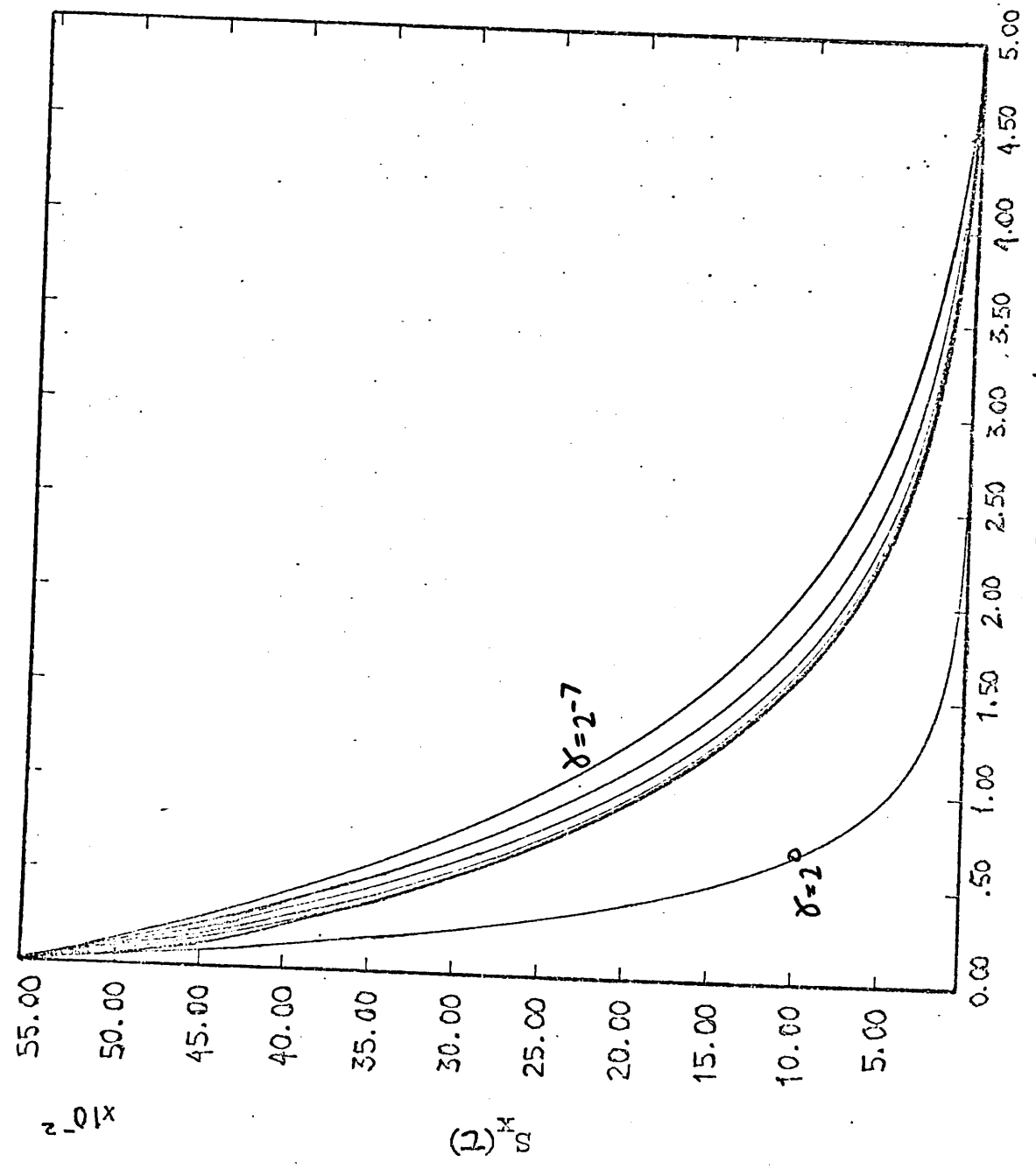
$$S_x(\tau) \sim (1/2).\exp(-4\gamma.\tau) \qquad (2.57)$$

with $\gamma = 2^{-7}$.

Electrical Conductivity

Figure 6 shows the real and imaginary parts of the complex admittance σ as functions of the frequency of the applied field. The results, plotted in dimensionless form in Figure 6

Figure 5


55.00
50.00
45.00
40.00
35.00
30.00
25.00
20.00
15.00
10.00
5.00
0.00
.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
5.00
τ-time scale
γ=2^-7
γ=2^0
x10^-2

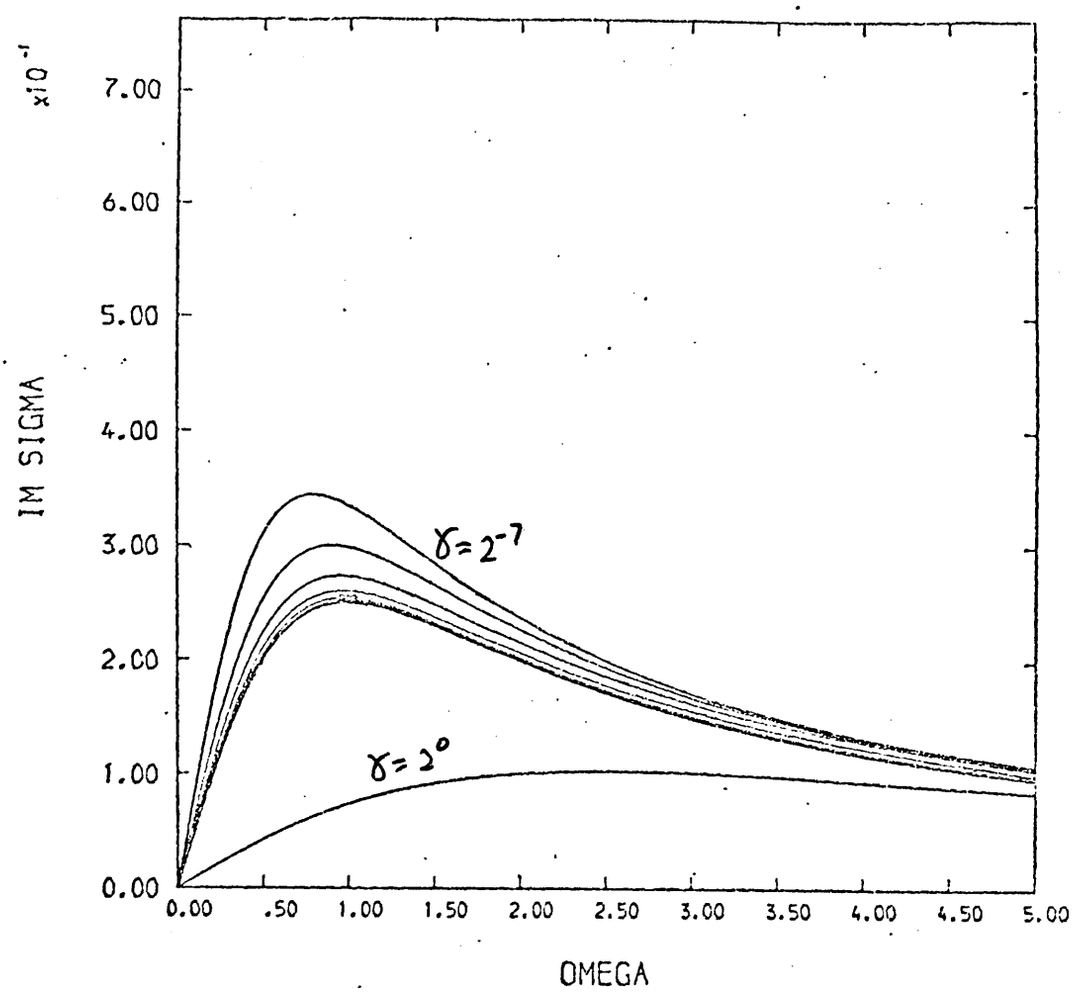
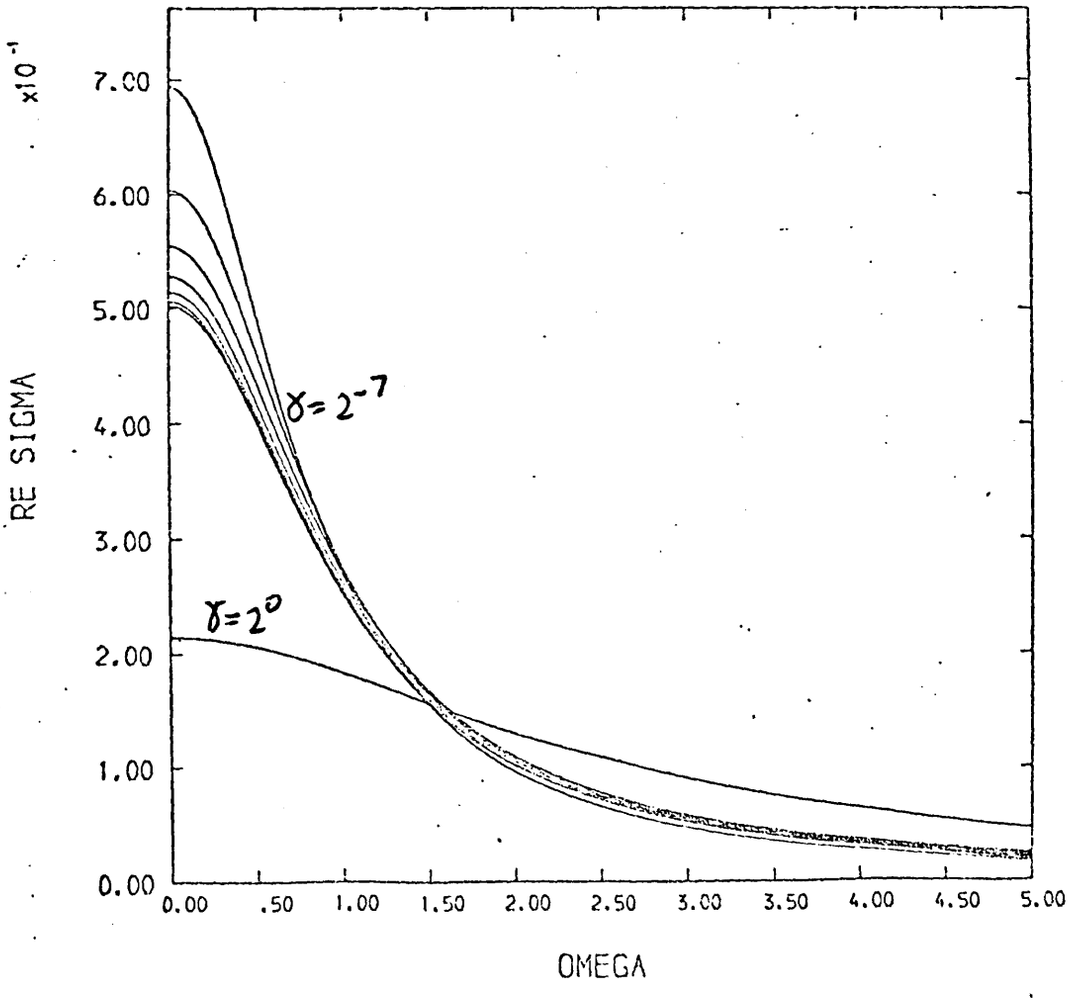

x10⁻¹
7.00
6.00
5.00
4.00
3.00
2.00
1.00
0.00
IM SIGMA
γ=2⁻⁷
γ=2⁰
0.00
.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
5.00
OMEGA

Figure 6


x10⁻¹
7.00
6.00
5.00
4.00
3.00
2.00
1.00
0.00
RE SIGMA
γ=2⁻⁷
γ=2⁰
0.00
.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
5.00
OMEGA

are seen to correspond broadly to physical intuition. Thus the dissipative component [Re.(σ)] representing the transmission of energy to the heat-bath, is maximum under dc conditions (and takes increasing values with decreasing mass ratio γ) and falls with a bell-shaped decay to zero at higher frequencies. There is no sign of resonance and frequencies much higher than the mean collision frequency are required for the dissipation to be effectively zero. The gamma-one curve decays very slowly relative to other curves.

CHAPTER THREE

SINGULAR EIGENFUNCTION SOLUTION OF THE SPECIAL MODEL

Section 3.1. Statistical Models In One Dimension

In one dimension the most extensively studied statistical dynamical model is probably the system of hard rods which can conveniently be called the Japsen model. Some of the properties of this model were considered by Frisch and others (Frisch 1956; Teramoto and Suzuki 1955). But the most detailed analysis, involving considerable mathematical ingenuity, was presented by Jepsen (1965). Later the model was studied by Lebowitz and Percus (1966) from the point of view of the kinetic equation and density expansion. Briefly the model can be described as an assembly of N hard rods, all of equal mass, constrained to move along a line like beads in an abacus. The rods do not penetrate each other, so that they retain their ordering along the line. When two rods collide, their energy and momentum are conserved so that they merely exchange velocities.

In order to study non-equilibrium systems, any realistic programme would naturally contain a 'fundamental statistical' assumption. For example, to obtain a deeper understanding of some of the phenomena associated with Brownian motion, Ford and others (1965) considered a chain of coupled harmonic oscillators, where the initial co-ordinates and momenta of the heat-bath 'oscillator-assembly' were assumed to be distributed according to the canonical ensemble.

Jepson (1965) assumed 'Poincare cycle-pseudostochastic' behaviour for the hard rod system and gave general formulae for the non-equilibrium properties. It was seen earlier that in the Rayleigh model the notional heat-bath particles were assumed to provide an aspect of molecular chaos with which the test-particles in form of 'Rayleigh Pistons' interacted and thus came to equilibrium.

An alternative to the Japsen model in one dimension is the special Rayleigh model. This model is the Rayleigh model with the parameter γ set equal to one and allowing for the possibility of heat-baths other then the Maxwellian. Although the hard rod system is a true N-body statistical model, nevertheless, by its very nature, it cannot lead to 'true' relaxation. But certain 'ergodic properties' can be studied quite conveniently. It is clear that given a set of velocities for the hard rods; the property of velocity exchange on collisions leads to the conclusion that the velocity distribution set must remain fixed for all time. But a single labelled test-particle must evolve according to some time dependent position-velocity distribution function. In this way, the labelled test-rod system admits both the time velocity relaxation and equilibrium fluctuations as well as giving a well defined approach to Brownian motion in the limit of very heavy system particles. Kuščer and Williams (1967) have pointed out the fundamental distinction between this two statistical models.

It must not be forgotten that the Rayleigh model is based on the Markovian assumption. In our view the

Lebowitz and Percus (1967) approach to the Japsen model provides the best connection between these two models. By considering the spatially homogeneous non-Markovian kinetic equation obtained by the authors and its expansion in powers of density, it is immediately apparent, that to the first order in density the equation describes a Markovian transport equation. This transport equation is precisely the Master equation for the special Rayleigh model. Strangely the authors do not seem to have considered the first-order solution. The whole of our problem consists in finding the exact solution of this first-order equation. In chapter five the corresponding spatially dependent equation is considered.

In this chapter the exact eigenfunctions of the singular integral equation for the special model have been found. These functions turn out to be a remarkable class of 'Schwartz distributions' forming a basis set for the expansion of more general initial conditions with 'non-L_2' character. By considering different heat-baths, a wide class of singular solutions can be found, satisfying the general orthogonality and completeness conditions. In all cases it is also possible to reduce the crucial pseudofunctions to more explicitly defined generalised functions.

Section 3.2. Special Rayleigh Model

We consider an ensemble of Rayleigh test-particles interacting with heat-bath particles of equal mass which provide the molecular chaos required for the relaxation process. The

heat-bath distribution is defined quite generally as $h_o(V)$ and normalised to unity. From our previous calculations for the gereral Rayleigh model the transition kernel can be written immediately as

$$K(V|V') = C\,|V-V'|\,h_o(V') \qquad (3.1)$$

The transport equation follows as

$$\frac{\partial P(V,t)}{\partial t} = C\,h_o(V)\int_{-\infty}^{\infty} dV'\,|V-V'|\,P(V',t) - Z(V).P(V,t) \qquad (3.2)$$

where the collision number function

$$Z(V) = C\int_{-\infty}^{\infty} dV'\,|V-V'|\,h_o(V') \qquad (3.3)$$

C is the frequency factor with dimensions $(\text{time})^{-1}.(\text{velocity})^{-1}$

In order to simplify the analysis it is convenient to introduce reduced variables. By analogy with the general problem, discussed in chapter two, the following scaled variables are introduced:

$$\begin{aligned} x &= V/\pi^{\frac{1}{2}}\bar{V}_o \\ y &= V'/\pi^{\frac{1}{2}}\bar{V}_o \\ \tau &= Z(0)t \end{aligned} \qquad (3.4)$$

where

$$\begin{aligned} Z(0) &= 2C\int_0^{\infty} Vh_o(V)dV \\ &= C\bar{V}_o \end{aligned} \qquad (3.5)$$

$\bar{V}_o$ is the mean speed. By introducing

$$P(x,\tau) = (\pi^{\frac{1}{2}}\bar{V}_o).\ P(\pi^{\frac{1}{2}}\bar{V}_o x,\ \tau/Z(0)) \qquad (3.6)$$

the transport equation in reduced variables becomes

$$\frac{\partial P(x,\tau)}{\partial \tau} = \hat{h}_o(x)\int_{-\infty}^{\infty} dy|x-y|P(y,\tau) - z(x)P(x,\tau) \qquad (3.7)$$

where by definition

$$\hat{h}_o(x) = \pi^{\frac{1}{2}} H_o(x)$$

$$= \pi^{\frac{1}{2}}.\ (\pi^{\frac{1}{2}}\bar{V}_o.\ h_o(\pi^{\frac{1}{2}}\bar{V}_o x)) \qquad (3.8)$$

Note that (3.7) represents a well defined transport equation with the probability conservation law:

$$\int_{-\infty}^{\infty} dx P(x,\tau) = \int_{-\infty}^{\infty} dx\ H_o(x) = \int_{-\infty}^{\infty} dx \hat{h}_o(x)/\pi^{\frac{1}{2}} = 1 \qquad (3.9)$$

The scaled transition kernel and the scaled collision function $z(x)$ are related by the relationship

$$z(x) = \int_{-\infty}^{\infty} dy\ k(x|y)$$

$$= \int_{-\infty}^{\infty} dy\ |x-y|\tilde{h}_o(y) \qquad (3.10)$$

Thus consistency with the reduced variables (2.14) in case of Maxwellian distribution has been maintained. It is worth noting that:

$$\hat{h}_o(x) > 0. \qquad -\infty < x < \infty$$

$$\hat{h}_o(-x) = \hat{h}_o(x)$$

$$z(o) = \int_{-\infty}^{\infty} y\, \hat{h}_o(y)\, dy = 1 \qquad (3.11)$$

$$z(x) \longrightarrow \pi^{\frac{1}{2}} x \quad \text{as} \quad x \longrightarrow \infty \qquad (3.12)$$

$$z'(x) = 2 \int_{o}^{x} \hat{h}_o(y) dy \qquad (3.13)$$

$$z''(x) = 2\hat{h}_o(x) \qquad (3.14)$$

To these we may add further obvious consequences

$$z(x) - xz'(x) \longrightarrow 0 \quad \text{as} \quad x \longrightarrow \infty \qquad (3.15)$$

$$z(x) = 1 + \hat{h}_o(o)x^2 + O(x^4) \qquad (3.16)$$

Section 3.3. Eigenvalue Problem

The symmetry properties of the kernel $k(x|y)$ play a crucial role in the physics of the model and for mathematical purposes. Using the relationship

$$|x-y| = \underbrace{\max(|x|, |y|)}_{\text{(even)}} - \underbrace{\operatorname{sgn}(x).\operatorname{sgn}(y).\min(|x|, |y|)}_{\text{(odd)}} \qquad (3.17)$$

(see figure 7) the transport equation (3.7) can be written in terms of the odd and even components. Using the decomposition:

$$P_{ev}(x,\tau) = (P(x,\tau) + P(-x,\tau))/2$$

$$P_{od}(x,\tau) = (P(x,\tau) - P(-x,\tau))/2 \qquad (3.18)$$

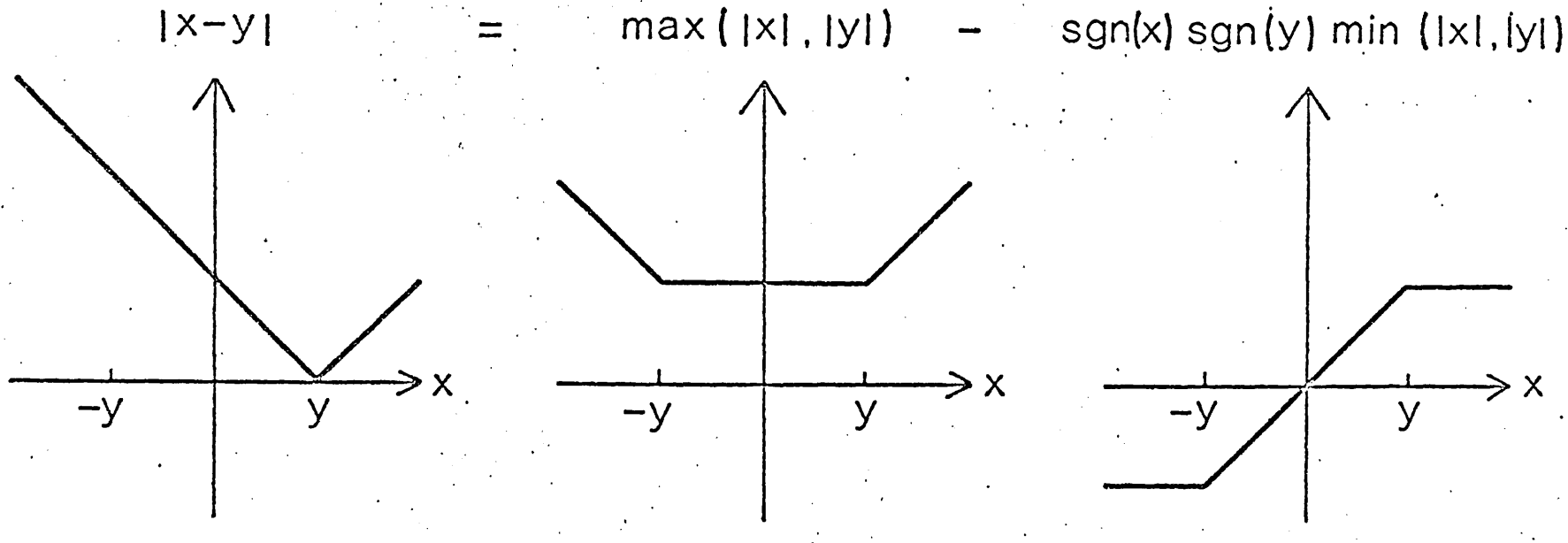


Figure 7

and the somewhat unfamiliar relationship (3.17) we have

$$\frac{\partial P_{ev}(x,\tau)}{\partial \tau} = 2\hat{h}_o(x)\int_o^\infty dy\, P_{ev}(y,\tau).\max(|x|, y) - z(x)P_{ev}(x,\tau) \qquad (3.19a)$$

and

$$\frac{\partial P_{od}(x,\tau)}{\partial \tau} = -2\mathrm{sgn}(x)\hat{h}_o(x)\int_o^\infty \min(|x|, y).P_{od}(y,\tau)dy - z(x)P_{od}(x,\tau) \qquad (3.19b)$$

The physical significance of the above is that whereas $P_{ev}(x,\tau) = P(|x|,\tau)/2$ is in effect the distribution function for <u>speeds</u> in the relaxing ensemble, the quantity $\phi(x,\tau) = |x|P_{od}(x,\tau)$ determines the <u>flux</u> of particles with speed in the range $d|x|$ about x at a given time. From this we obtain by integration, the net flux $\phi(\tau)$ as a function of time

$$\phi(\tau) = 2\int_o^\infty xP_{od}(x,\tau) \qquad (3.20)$$

$$= \langle x(\tau)\rangle$$

(Note that positive values indicate an excess current to the right, negative to the left). As indicated, this quantity is identical in one dimension with the time-dependent mean-velocity. The heat-bath distribution being strictly <u>even</u>, all

the above quantities related to P_{od} must decay to zero at infinite time.

The Maxwellian Heat-bath

For later reference, and to connect with our earlier work (Hoare and Rahman 1973/74) we may summarise here the special forms taken by the above relationships in case of the Maxwellian heat-bath. Given the Gaussian velocity distribution $\hat{h}_o(x) = \exp(-x^2)$, we have

$$z(x) = \exp(-x^2) + \pi^{\frac{1}{2}} x \, \mathrm{erf}(x) \qquad (3.21)$$

$$z'(x) = \pi^{\frac{1}{2}} \mathrm{erf}(x) \qquad (3.22)$$

$$z''(x) = 2 \exp(-x^2) \qquad (3.23)$$

It may be noted that, for the Maxwellian case alone we have the strict identity:

$$z(x) = z''(x)/2 + xz'(x) \qquad (3.24)$$

The following properties may also be seen to be independent of the particular specification of the heat-bath distribution.(As we have seen in chapter one the first property below is necessary in order to cast the eigenvalue problem into self-adjoint form (see (1.26)) .)

(a) The kernel satisfies detailed balance condition for reversed collisions:

$$\hat{h}_o(x).k(x|y) = \hat{h}_o(y).k(y|x) \qquad (\ 3.25\ )$$

(b) The kernel satisfies inverse collision symmetry:

$$k(x|-y) = k(-x|y) \qquad (\ 3.26\ )$$

(c) The function $\hat{h}_o(x)$, by virtue of (a) above satisfies equation (3.7) with left hand side zero. Thus $P(x,\infty) = H_o(x)$ is a time independent solution for the equilibrium ensemble. This evidently corresponds to the eigenvalue $\lambda_o = 0$

(d) The spectrum divides into regular and singular branches. The singular brach, corresponding to non-L_2 eigenfunctions, may fill the interval $(1,\infty)$, the totality of points for which there exists roots $\pm x_\lambda$ satisfying $z(\pm x_\lambda) = \lambda$.

(e) <u>The Discrete Spectrum</u>

The eigenvalue problem of equation (3.7) follows by the substitution

$$P(x,\tau) = f(x,\lambda)\exp(-\lambda\tau) \qquad (\ 3.27\ )$$

$$(\ z(x) - \lambda)f(x,\lambda) = \hat{h}_o(x) \int_{-\infty}^{\infty} dy\,|x-y|\,f(y,\lambda) \qquad (\ 3.28\ )$$

In order to prove the emptiness of the discretum, it is convenient to work with the following unsymmetric equation, obtained by substituting

$$f(x,\lambda) = \hat{h}_o(x)\phi(x,\lambda) \qquad (\ 3.29\ )$$

in equation (3.7):

$$(z(x) - \lambda)\phi(x,\lambda) = \int_{-\infty}^{\infty} dy\,|x-y|\,\phi(y,\lambda)\hat{h}_o(y) \qquad (3.30)$$

On differentiating the above equation twice and using the identity

$$\frac{d^2}{dx^2}\,|x-y| = 2\delta(x-y) \qquad (3.31)$$

we have

$$(z(x) -\lambda)\phi''(x,\lambda) + 2z'(x)\phi'(x) = 0 \qquad (3.32)$$

So long as $\lambda < 1$ this is an elementary equation with the general solution:

$$\phi(x,\lambda) = A\int_{o}^{x} dy/(z(x)-\lambda)^2 \quad + \quad B \qquad (3.33)$$

The boundary conditions can be recovered from the integral equation (3.30) and its once differentiated form:

$$z'(x)\phi(x,\lambda) + \phi'(x).(z(x)-\lambda) = \int_{-\infty}^{\infty} dy\,sgn(x-y).\tilde{h}_o(y)\phi(y,\lambda) \qquad (3.34)$$

By setting x = 0 in (3.30) and (3.34) one obtains

$$(1-\lambda)\phi(o,\lambda) = \int_{-\infty}^{\infty} dy\,|y|\hat{h}_o(y).\phi(y,\lambda) \qquad (3.35a)$$

$$(1-\lambda)\phi'(o,\lambda) = -\int_{-\infty}^{\infty} dy\,sgn(y)\tilde{h}_o(y)\phi(y,\lambda) \qquad (3.35b)$$

Recognising that the terms in A and B are odd and even components of the solution respectively, we obtain the conditions

$$(1-\lambda)B = B \qquad (3.36a)$$

$$A/(1-\lambda) = A/(1-\lambda) - A\, z'(\infty) \int_0^\infty dy/(z(y)-\lambda)^2 \qquad (3.36b)$$

where we had to use the relatioship:

$$2\int_0^\infty dy\hat{h}_0(y) \int_0^y \frac{dx}{(z(x)-\lambda)^2} = z'(\infty)\int_0^\infty \frac{dy}{(z(y)-\lambda)^2} - \frac{1}{(1-\lambda)} \qquad (3.37)$$

From above it follows that $A=B=0$ if $\lambda \neq 0$ or B is arbitrary and $A=0$ if $\lambda=0$. (Hoare and Rahman 1973/74). Hence the discretum is empty except for $\lambda=0$ eigenvalue, which corresponds to the equilibrium distribution. The singular eigenfunctions are considered in section five.

Section 3.4. The Singular Eigenfunctions: Case's Method

For those not familiar with singular integral equations it is probably necessary to point out the singular nature of the eigenvalue problem (3.30). These equations may be treated with the well known method, which , introduced by Carleman in a particular case in 1922, were remarkably generalised and standardised in a monograph by N.I.Mushkhelishvili (1953). In this monograph, only the singular equations involving Cauchy principal values were examined, hence it is natural to call this the theory of Cauchy singular integral equations.

In 1960, Case presented an interesting method for handling problems connected with the neutron transport equation. In the paper, he demonstrated that the typical problems of neutron transport theory can be solved by finding a complete set of 'elementary solutions' consisting of distributions. The general solution then follows by superposition of these solutions and by imposing boundary conditions. Zelazny, Kuszell amd Mika (1960) have successfully applied the method to other problems, namely, the solution of the criticality problem with anisotropic scattering. The results of this applications seem to be satisfactory provided that the investigated equation does not differ too much from the one-speed transport equation treated by Case (1960). (In essence the equation is always of Cauchy singular integral type.)

The basic principles are quite straightforward and can be illustrated by considering the homogeneous one-speed transport equation. It is not intended here to repeat all the steps of the proof but rather to present a brief description of the method. (The standard reference to linear transport theory is a monograph by K.M.Case and P.F.Zweifel 1967.) This will serve the following useful purposes:

(i) The description will give the reader an impression of the method.
(ii) Equation (3.19) will be solved by looking for 'elementary solutions' by analogy with Case's method.
(iii) All the comments one can make about the validity of the procedure for solving the one-speed transport equation apply

equally to the method of solving equation (3.19) by the singular eigenfunction method.

(iv) Thus we shall be in a position to understand the difficulties involved in solving equation (3.19) by the singular eigenfunction method.

The one-speed homogeneous linear transport equation is

$$\mu\frac{\partial\psi(x,\mu)}{\partial x} + \psi(x,\mu) = c/2.\int_{-1}^{+1} d\mu'\psi(x,\mu') \qquad (3.38)$$

where x is a real variable and μ ranges over the interval $-1 \leq \mu \leq +1$. By separation of variables in the form:

$$\psi(x,\mu) = X(x).\phi(\mu) \qquad (3.39)$$

the problem reduces to the pair of equations:

$$(\nu-\mu)\phi_\nu(\mu) = c/2\ \nu\int_{-1}^{+1}\phi_\nu(\mu')d\mu' \qquad (3.40)$$

$$\frac{\partial X_\nu}{\partial x} = -X_\nu/\nu \qquad (3.41)$$

A possible solution is assumed to be normalised by

$$\int_{-1}^{+1}\phi_\nu(\mu')d\mu' = 1 \qquad (3.42)$$

provided that the left-hand side does not vanish. Apart from a constant factor, equation (3.41) has a solution

$$X_\nu = \exp(-x/\nu) \qquad (3.43)$$

and equation (3.40) becomes

$$(\nu-\mu)\,\phi_\nu(\mu) = c/2\,\nu \qquad (3.44)$$

Now there are two possibilities:

(a) If ν does not lie between -1 and +1 on the real line then

$$\phi_\nu(\mu) = c/2\,.(\,\nu/(\nu-\mu)\,) \qquad (3.45)$$

The normalisation condition yields two solutions ($c \neq 1$)

$$\Psi_{o\pm}(x,\mu) = \phi_{o\pm}(\mu)\exp(\mp\, x/\,\nu_o\,) \qquad (3.46a)$$

where

$$\phi_{o\ \pm}(\mu) = \frac{c}{2}\cdot\frac{\nu_o}{(\nu_{o\mp}\,\mu)} \qquad (3.46b)$$

(b) If ν is a real number between -1 and +1 then

$$\phi_\nu(\mu) = \frac{c}{2}\,P.\frac{\nu}{\nu-\mu} \quad + \lambda(\nu).\delta\,(\nu-\mu) \qquad (3.47)$$

where P.1/x indicates the distribution 'principal part of 1/x'. The constant $\lambda(\nu)$ is determined by the normalisation condition (3.42):

$$\lambda(\nu) = 1- \frac{c}{2}\,\nu \int_{-1}^{+1} d\mu/(\nu-\mu) \qquad (3.48)$$

Then

$$\Psi_\nu(x,\mu) = \phi_\nu(\mu)\exp(-x/\nu) \qquad (3.49)$$

The solutions (3.46) and (3.47) are called eigenfunctions 'in analogy with ordinary terminology'. The corresponding values of ν are called discrete and continnum eigenvalues.

Next, orthogonality and completeness theorems for the eigenfunctions are proved, and their normalisation is obtained.

(i) Orthogonality:

Follows quite simply if we use the proof presented in chapter one (1.39)

$$\left[\frac{1}{\nu'} - \frac{1}{\nu}\right] \cdot \int_{-1}^{+1} \mu \phi_{\nu}(\mu)\, \phi_{\nu'}(\mu) d\mu \qquad (3.50)$$

Note that the proof involves product of distributions.

(ii) Normalisation

The normalisation integral is the value of the integral in (3.50) when $\nu = \nu'$. For the discrete eigenvalues no difficulties arise in the definition or the computation. To make the discussion clear we quote from ' Linear Transport Theory' by K.M.Case and P.F.Zweifel (1967) (see page 69.):

"To obtain normalisation integral for the continuum modes, it is necessary to proceed with more care, since the distribution functions which appear in the continuum eigenfunctions are not square integrable. However, it is possible to define normalisation integrals in the following sense:

We wish to use the normalisation integrals to evaluate the the coefficients in the expansion of an arbitrary function $f(\mu)$

$$f(\mu) = \int_{-1}^{+1} A(\nu') \phi_{\nu'}(\mu) d\nu' \qquad (9)$$

Multiplying by $\mu \phi_{\nu}(\mu)$ and integrating we find that

$$\int_{-1}^{+1} \mu\phi_\nu(\mu) f(\mu) d\mu = \int_{-1}^{+1} \mu\phi_\nu(\mu) \int_{-1}^{+1} A(\nu')\phi_{\nu'}(\mu) d\nu' \, d\mu \qquad (10)$$

Then the left hand side of equation (10) is defined, in analogy with the usual case, to be the product of $A(\nu)$ with the normalisation constant $N(\nu)$. Thus

$$N(\nu) = \frac{1}{A(\nu)} \cdot \int_{-1}^{+1} \mu\phi_\nu(\mu) \; A(\nu')\phi_{\nu'}(\mu) d\nu' \, d\mu \qquad (11)$$

We have emphasised this point because this is one of those rare situations in physics, in which the order of integration is important (because of the singular nature of the functions $\phi_\nu(\mu)$.)....."

By using the Poincare'- Bertrand formula the above double integral is evaluated and the following relationship is ascertained:

$$\int_{-1}^{+1} d\mu \; \mu \; \phi_{\nu'}(\mu)\phi_\nu(\mu) = N(\nu)\delta(\nu-\nu') \qquad (3.51)$$

where $N(\nu) = \nu(\lambda^2(\nu) + (\pi c\nu/2)^2)$. This relationship is said to be <u>symbolic</u>.

(iii) <u>Completeness</u>

A proof is given that a function $\phi(\mu)$, which satisfies some suitable Hölder conditions, can be written in the form:

$$\phi(\mu) = a_{o+}\phi_{o+}(\mu) + a_{o-}\phi_{o-}(\mu) + \int_{-1}^{+1} A(\nu)\phi_\nu(\mu) d\nu \qquad (3.52)$$

where a_{o+}, a_{o-} and $A(\nu)$ are expansion coefficients. $A(\nu)$ is

presumed to satisfy suitable Hölder conditions. These expansion coefficients are found by inserting (3.47) in formula (3.52) and considering the resulting equation to be a singular integral equation for the unknown function $A(\nu)$. (Which is solved by methods given in the monograph by N. I. Mushkhvili 1953.) Once it can be proved that $A(\nu)$ exists , then the orthogonality property can be used to find the acutal expression for $A(\nu)$. For example

$$A(\nu) = \frac{1}{N(\nu)} \cdot \int_{-1}^{+1} d\mu \; \mu \phi_\nu(\mu) \phi(\mu) \qquad (3.53)$$

where $N(\nu)$ is the function given in (3.51).

At this point, having presented Case's method in outline only, we quote from Hagelbroek's thesis (1973) all the objections he raises against Case's method.

"(i) The choise of the additional solutions $\lambda(\nu)\delta(\nu-\mu)$ of equation (3.44) in case $-1 < \nu < +1$ is quite arbitrary. The reason for this choice seems to be that equation (3.44) as an equation for an unknown distribution admits the solution written down above. But it does not seem clear why one has to have recourse to distribution theory.

(ii) The eigenfunctions ϕ_ν given in (3.47) have been obtained for fixed values of ν amd make sense only if they are applied to functions of μ. It seems surprising that they can be applied to functions of ν for fixed values of μ.

(iii) The relations (3.50) and (3.51), and also the procedure by which these relations are obtained are quite embarrasing since the product of distributions has not been defined.

(iv) The function μ appears many times in expressions which look like inner products (cf. (3.51), (3.53)). The function μ is called in these cases a weight function by Case and others, though it is not non-negative definite. It is surprising that such a weight function does not give rise to serious difficulties.

(v) The completeness of the set of eigenfunctions ϕ_ν is proved for functions which satisfy suitable Hölder conditions, but an expansion of the type (3.52) is also given and used for the delta function.

(vi) It is tacitly assumed that, given b and $B(\nu)$ ($\psi(x,\mu) = b_{o+}\psi_{o+}(x,\mu)+b_{o-}\ _{o-}(x,\mu)+ \int B(\nu)\ _\nu(x,\mu)d\nu$), the function $\psi(x,\mu)$ will be itself a solution of equation (3.38). "

Hagelbroek did not deny the results obtained by the method, his objective was to make the method more rigorous. In the next section the method is applied to find the solution of equation (3.19). The objections raised above will naturally apply to the solution obtained below.

Section 3.5. Singular Eigenfunctions of the Special Model

(A) Eigenvalue Equations

As we have outlined above, the solutions of eigenvalue equations, corresponding to the uncoupled transport equation (3.7),

$$(z(x) -\lambda)\phi_{ev}(x,\lambda) = 2\int_o^\infty dy \max(|x|, y)\hat{h}_o(y)\phi_{ev}(x,\lambda) \qquad (3.54)$$

and

$$(z(x)-\lambda)\phi_{od}(x,\lambda) = -2\mathrm{sgn}(x)\int_0^\infty dy \min(|x|,y)\hat{h}_o(y)\phi_{od}(y,\lambda) \qquad (3.55)$$

obtained by making the substitution

$$P_{ev}(x,\tau) = \hat{h}_o(x)\phi_{ev}(x,\lambda)\exp(-\lambda\tau) \qquad (3.56)$$

in (3.19a) and

$$P_{od}(x,\tau) = \hat{h}_o(x)\phi_{od}(x,\lambda)\exp(-\lambda\tau) \qquad (3.57)$$

in (3.19b), while radically altered in the continuum $\lambda > 1$, may nevertheless be interpreted satisfactorily within the realm of generalised functions. Recalling that the generalised solution to

$$x^n F(x) = 1 \qquad (3.58a)$$

is

$$F(x) = \mathrm{pf}.1/x^n + \sum_{k=0}^{n-1} a_k \delta^k(x) \qquad (3.58b)$$

where $\delta^k(x)$ is the k^{th} derivative of the delta function and Pf. designates the pseudofunction corresponding to the Hadamard finite part of the implied divergent integral. More explicitly, we understand the action of the pseudofunction above through the functional:

$$\langle \mathrm{Pf}.1/x^n, \phi(x)\rangle = \mathrm{Fp}.\int_{-\infty}^{\infty} dx\phi(x)/x^n \qquad (3.59)$$

where $\phi(x)$ is a test function (For details see the standard

references cited earlier on the theory of distributions and Appendix C.)

Differentiating equations (3.54) and (3.55) once, one obtains the following pair of equations:

$$(z(x) -\lambda)\phi'_{ev}(x,\lambda) + z'(x)\phi_{ev}(x,\lambda) = 2\int_0^x dy\hat{h}_o(y)\phi_{ev}(y,\lambda) \qquad (3.60)$$

$$(z(x) -\lambda)\phi'_{od}(x,\lambda) + z'(x)\phi_{od}(x,\lambda) = -2\int_x^\infty dy\hat{h}_o(y)\phi_{od}(y,\lambda) \qquad (3.61)$$

Differentiating the above pair of equations we obtain

$$F''(x,\lambda)(z(x)-\lambda) + 2z'(x)F'(x) = 0 \qquad (3.62)$$

where $F(x,\lambda)$ is either $\phi_{ev}(x,\lambda)$ or $\phi_{od}(x,\lambda)$. The above equation can, more conveniently, be written in the form:

$$\frac{d(z(x)-\lambda)^2F'(x)}{dx} = 0 \qquad (3.63)$$

Now if $\hat{G}(x)$ is a distribution then $\hat{G}'(x) = 0$ has only the solution $\hat{G}(x) =$ constant i.e. the classical solution (see e.g. Jones 1966 page 89.). Therefore, from the above equation it follows that

$$(z(x)-\lambda)^2 \phi'_{ev}(x,\lambda) = A_1 \qquad (3.64)$$

and

$$(z(x)-\lambda)^2\phi'_{od}(x,\lambda) = A_2 \qquad (3.65)$$

where A_1 and A_2 are constants.

(B) The Even Eigenfunctions

We know that $\phi'_{ev}(x,\lambda)$ must be odd function. Therefore, the constant $A_1 = 0$ and the solution of (3.64) can be written as

$$\phi'_{ev}(x,\lambda) = B_1(\delta(x-|x_\lambda|)- \delta(x+|x_\lambda|)) + C_1(\delta'(x-|x_\lambda|)+ \delta'(x+|x_\lambda|)) \qquad (3.66)$$

(Throughout prime denotes differentiation with respect to x.)
The identity

$$\delta(z(x)-\lambda) = \frac{1}{|z'(x_\lambda)|}(\delta(x-|x_\lambda|) + \delta(x+|x_\lambda|)) \qquad (3.67)$$

has been used above. It only holds if $|x_\lambda| \neq 0$. From above by integration we have

$$\phi_{ev}(x,\lambda) = A + B_1(H(x-|x_\lambda|)+H(-x-|x_\lambda|)) + C_1(\delta(x-|x_\lambda|)+\delta(x+|x_\lambda|)) \qquad (3.68)$$

where $H(x-y)$ is the Step-function and A, B_1, and C_1 are integration constants.

In order to find these constants, we

substitute the solution in the original equation (3.54) and (3.63). By setting x=o in (3.54) we obtain

$$(1-\lambda)A = 2\int_o^\infty dy \hat{h}_o(y)\phi_{ev}(y,\lambda)$$

$$= A + B_1(z(x_\lambda)-x_\lambda z'(x_\lambda)) + 2|x_\lambda| \hat{h}_o(x_\lambda)C_1 \qquad (3.69)$$

And from (3.63) after lengthy calculations

$$B_1 z'(|x_\lambda|) = C_1 z''(x_\lambda) \qquad (3.70)$$

By solving in terms of A the even solution becomes

$$\phi_{ev}(x,\lambda) = A \left[1-(H(x-|x_\lambda|)+H(-x-|x_\lambda|)) + q(x_\lambda).(\delta(x-|x_\lambda|)+\delta(x+|x_\lambda|)) \right] \qquad (3.71)$$

where $q(x_\lambda) = |z'(x_\lambda)| / z''(x_\lambda)$ (3.72)

The single normalisation constant remains to be determined.

(C) The Odd Eigenfunctions

From equation (3.65)

$$\phi'_{od}(x,\lambda) = Pf.\frac{A_2}{(z(x)-\lambda)^2} + B_2(\delta(x-|x_\lambda|)+\delta(x+|x_\lambda|)) + C_2(\delta'(x-|x_\lambda|)-\delta'(x+|x_\lambda|)) \qquad (3.73)$$

because $\phi'_{od}(x,\lambda)$ must be even function in x. By integration

$$\phi'_{od}(x,\lambda) = A_2 R(x,\lambda) + B_2\left(H(x-|x_\lambda|)-H(-x-|x_\lambda|) \right)$$

$$+ C_2\left(\delta(x-|x_\lambda|)-\delta(x+|x_\lambda|) \right) \qquad (3.74)$$

where

$$R(x,\lambda) = \text{Pf.} \int_0^x dy/(z(y)-\lambda)^2 \qquad (3.75)$$

In order to find the constants of integration B_2 and C_2, we have substituted in equation (3.55) and (3.63) the above expression for $\phi_{od}(x,\lambda)$. By setting x=o we obtain:

$$A_2/(1-\lambda) = -2\int_0^\infty dy\hat{h}_o(y)A_2R(y,\lambda) -2B_2 \int_{|x_\lambda|}^\infty dy\hat{h}_o(y) - 2C_2\hat{h}_o(x_\lambda)$$

(3.76)

And from equation (3.63) after lengthy calculations:

$$B_2 z'(|x_\lambda|) = C_2\, z''(x_\lambda) \qquad (3.77)$$

By using the identity

$$2\int_0^\infty dy\hat{h}_o(y)R(y,\lambda) = z'(\infty)R(\infty,\lambda)- 1/(1-\lambda) \qquad (3.78)$$

(see Appendix C) equation (3.76) becomes:

$$-A_2 z'(\infty)R(\infty,\lambda) = B_2.(z'(\infty)- z'(|x_\lambda|)) + 2C_2\hat{h}_o(x_\lambda)$$

(3.79)

By solving in terms of A_2 the odd solution becomes:

$$\phi_{od}(x,\lambda) = A_2\Big[R(x,\lambda) - R(\infty,\lambda).\big(H(x-|x_\lambda|)-H(-x-|x_\lambda|)\big)$$

$$-R(\infty,\lambda)q(x_\lambda).\big(\delta(x-|x_\lambda|)-\delta(x+|x_\lambda|)\big)\Big]$$

(3.80)

$q(x_\lambda)$ is defined by equation (3.72) and the normalisation constant A_2 still remains to be determined.

We are now in the stage of Case's method where $\phi_\nu(\mu)$ had been determined for all values of ν. The reader will have noticed the complexity of the expressions involved in the above singular eigenfunctions. The properties of the pseudofunction $R(x,\lambda)$ have been looked at in detail in Appendix C (Hoare and Rahman 1974).

(D) The Special Case $x_\lambda = o$

It is very important to realise that the above expressions for $\phi_{ev}(x,\lambda)$ and $\phi_{od}(x,\lambda)$ hold only if $|x_\lambda| > o$, where $\lambda = z(\pm x_\lambda)$. If we recognise the identity

$$1-\big(H(x-|x_\lambda|)+H(-x-|x_\lambda|)\big) = H(x+|x_\lambda|)-H(x-|x_\lambda|)$$

(3.81)

then the even eigenfunctions can be written in the form:

$$\phi_{ev}(x,\lambda) = A\big(H(x+|x_\lambda|)-H(x-|x_\lambda|)$$

$$-q(x_\lambda).\{\delta(x-|x_\lambda|)+\delta(x+|x_\lambda|)\}\big)$$

(3.82)

It is evident from above that $\phi_{ev}(x,o)=0$. Later it has been proved that the result holds also for the odd eigenfunctions with the consequence that the singular branch of the spectrum is the open interval $(1,\infty)$ rather than the closed interval $[1,\infty)$. For general singular eigenvalue problems of the type we are considering, it is conceivable that the singular branch could be of the form (a,b) or $[a,b)$ or $(a,b]$ or $[a,b]$. A point rarely recognised in the standard literature.

(E) Orthogonality Property

The orthogonality property of the eigenfunctions is guaranteed as we have seen in chapter one (1.24) by the detailed balance condition (1.22) which is used to find the self adjoint integral equation (1.26).

Nevertheless, because the orthogonality relationship involves products of distributions, it is worthwhile to present a direct proof of the relationship. The symmetric integral equation corresponding to equation (3.28) has eigenfunctions of the form (see (1.30)):

$$\Phi(x,\lambda) = (\hat{h}_o(x))^{\frac{1}{2}}\phi(x,\lambda) \qquad (3.83)$$

We would like to prove that the set $((h_o(x))^{\frac{1}{2}}, \Phi_{ev}(x,\lambda) , \Phi_{od}(x,\lambda))$ forms an orthogonal system. This is proved in Appendix C by calculation of the following integrals:

$$I_1 = \int_{-\infty}^{\infty} dx\, \hat{h}_o(x)\, \phi_{ev}(x,\lambda)\phi_{ev}(x,\lambda') = A(\lambda)^2 N_1(\lambda)\delta(\lambda-\lambda') \qquad (3.84)$$

where $N_1(\lambda) = \dfrac{|z'(x_\lambda)|^3}{z''(x_\lambda)}$.

$$I_2 = \int_{-\infty}^{\infty} dx \hat{h}_o(x) \phi_{od}(x,\lambda) \phi_{od}(x,\lambda') = A_2(\lambda)\, N_2(\lambda) \delta(\lambda-\lambda') \qquad (3.85)$$

where $N_2(\lambda) = R(\infty,\lambda).\ N_1(\lambda)$

$$I_3 = \int_{-\infty}^{\infty} dx \hat{h}_o(x) \phi_{ev}(x,\lambda) = 0 \qquad (3.86)$$

and from the parity property of the above eigenfunctions

$$I_4 = \int_{-\infty}^{\infty} dx \hat{h}_o(x) \phi_{od}(x,\lambda) = 0 \qquad (3.87)$$

$$I_5 = \int_{-\infty}^{\infty} dx \hat{h}_o(x) \phi_{ev}(x,\lambda) \phi_{od}(x,\lambda') = 0 \qquad (3.88)$$

There is a fundamental difference between the normalisation integral (3.51) and the orthogonal integrals I_1 and I_2. The former is purely a symbolic relationship and the latter is obtained by actual multiplication and integration.

(F) The Completeness Property

The problem of completeness of the orthogonal set of functions above, like that for other singular solutions in transport theory is by no means clear-cut. It is not at all evident precisely what space is acually spanned by the singular

eigenfunctions $\bar{\Phi}(x,\lambda)$, though for practical purposes, a space including all ' reasonable ' probability distributions will be quite adequate. It is evident, nevertheless, that the space spanned by the set ($\bar{\Phi}_0(x)$, $\bar{\Phi}(x,\lambda)$), where $\bar{\Phi}_0(x) = \hat{h}_0(x)^{\frac{1}{2}}$, is more extensive than $L_2(-\infty,\infty)$ and certainly includes singular distributions equivalent to $\delta(x-x_0)$ and probably functions in $L_p(-\infty,\infty)$ with $p \geqslant 1$.

The procedure, as has been explained earlier, is to consider the unknown function spaces D_1 and D_2 spanned by the odd and even singular solutions, with a view to giving a constructive proof of completeness over any given class of functions. The next section is completely devoted to this problem.

Section 3.6. The Completeness Problem for the Eigenfunctions

(i) Completeness for the Even Eigenfunctions

Let $g(x)$ be an arbitrary function ($g(x) \varepsilon D_2$). Then there shall exists a coefficient a_0 and a function $a(\lambda)$ such that

$$g(x) = a_0\bar{\Phi}_0(x) + \int_1^{\infty} a(\lambda)\bar{\Phi}_{ev}(x,\lambda)\hat{h}_0(x)^{\frac{1}{2}}d\lambda \qquad (3.89)$$

As we shall always be interested in initial value problems where after a long time $P(x,\tau)$ must tend to $\hat{h}_0(x)/\pi^{\frac{1}{2}}$, it is convenient to consider only the component of $g(x)$ orthogonal to the heat-bath distribution:

$$g(x) = \hat{h}_o(x)/\pi^{\frac{1}{2}} + \int_1^{\infty} d\lambda a(\lambda)\hat{h}_o(x)\phi_{ev}(x,\lambda) \qquad (3.90)$$

where by definition

$$\int_{-\infty}^{\infty} dx(g(x) - \hat{h}_o(x)/\pi^{\frac{1}{2}}) = 0. \qquad (3.91)$$

By substituting the value of $\phi_{ev}(x,\lambda)$ in (3.90) and dividing throught by $\hat{h}_o(x)$, the following equation is obtained

$$f(x) = \int_{|x|}^{\infty} dx_\lambda \; \omega_1(x_\lambda)z'(x_\lambda) - \frac{z'(x)\omega_1(x)}{z''(x)} + 1/\pi^{\frac{1}{2}} \qquad (3.92)$$

where $f(x)=g(x)/\hat{h}_o(x)$ and $\omega_1(x) = A(x)a(x)$.
A transformation from the expansion parameter λ to x_λ has been made with the consequence that $\omega_1(x) = +\omega_1(-x)$. By differentiating the above equation with respect to x the following First-Order differential equation is obtained:

$$\frac{d\omega_1(x)}{dx} + P(x)\omega_1(x) = Q(x) \qquad (3.93)$$

where $$P(x) = \frac{d}{dx}\left(\mathrm{Ln}(|z'(x)|^3/z''(x)) \right)$$ and

$$Q(x) = -f'(x)z''(x)/z'(x)^2$$

The solution of equation (3.93) follows, from the standard theory of differential equations, as

$$\omega_1(x) = \frac{z''(x)}{z'(|x|)^3}\left[\int_0^{|x|} dx_\lambda z''(x_\lambda)f(x_\lambda) - z'(|x|)f(x) + \beta \right] \qquad (3.94a)$$

After substituting $\omega_1(x)$ in (3.92) , the integration constant β is found to be zero. Hence,

$$\omega_1(x) = \frac{z''(x)}{z'(|x|)^3}\left\{ 2\int_0^{|x|} dx_\lambda g(x_\lambda) - z'(|x|)g(x)/\hat{h}_o(x)\right\} \quad (3.94b)$$

Thus to find $\omega_1(x)$, only the simple integrability of the function $g(x)$ is required. The orthogonality of $\phi_{ev}(x,\lambda)$ distributions is expressed by the integral I_1 (3.84). If it is assumed that the order to integration (see below) can be exchanged then from (3.90) it follows that:

$$\int_{-\infty}^{\infty} dx g(x)\phi_{ev}(x,\lambda) = \int_{-\infty}^{\infty} dx \phi_{ev}(x,\lambda)\hat{h}_o(x) \cdot \int_1^{\infty} d\lambda' a(\lambda')\phi_{ev}(x,\lambda')$$

$$= \int_1^{\infty} d\lambda' a(\lambda').I_1$$

$$= A(\lambda)^2 N_1(\lambda) a(\lambda) \quad (3.95)$$

If we integrate the expression on the left hand-side above, it can be proved that the same expression as above for $\omega_1(x)$ is obtained. Therefore, by actual construction, we have not only proved that the even eigendistributions form a complete set but it also follows that the normalisation integral can be defined by using the orthogonality integral I_1 .

The set of distributions($\Phi_o(x), \Phi_o(x)\phi_{ev}(x,\lambda)$) where $\Phi_o(x) = \hat{h}_o(x)^{\frac{1}{2}}$ and

$$\phi_{ev}(x,\lambda) = N_1(x_\lambda)^{-\frac{1}{2}}.\Big[\; H(x+|x_\lambda|) - H(x-|x_\lambda|) - q(x_\lambda).\left(\delta(x-|x_\lambda|) + \delta(x+|x_\lambda|)\right)\Big] \qquad (3.96)$$

($q(x_\lambda) = z'(|x_\lambda|)/z''(x_\lambda)$), forms a complete orthonormal basis set. The orthonormalisation integral is given by:

$$\int_{-\infty}^{\infty} dx \hat{h}_o(x)\phi_{ev}(x,\lambda')\phi_{ev}(x,\lambda) = \delta(\lambda-\lambda') \qquad (3.97)$$

(ii) The Completeness for the Odd Eigenfunctions

Hoare and Rahman (1974) found that the proof of completeness condition for the odd eigendistributions was troublesome and could only be proved in terms of the solution of the Carleman equation (Tricomi 1957). The proof required strong assumptions about the interchangebility of integrals. In chapter four, the completeness property is proved by the method of Laplace transform in a straightforward way.

Nevertheless, it is worth attempting to prove the property by a direct method. Let $g_1(x)$ be an arbitrary function ($g_1(x) \in D_1$). Then it is asserted that a coefficient $b(\lambda)$ must exist, such that:

$$g_1(x) = \hat{h}_o(x)^{\frac{1}{2}} \int_1^{\infty} d\lambda b(\lambda)\phi_{od}(x,\lambda) \qquad (3.98)$$

As we shall always be interested in initial value problems, it

is convenient to consider $g_2(x) = g_1(x).h_o(x)^{\frac{1}{2}}$. By substituting $\phi_{od}(x,\lambda)$ in (3.98) and defining $\omega_2(x) = A_2(x)b(x)$, we have

$$g_2(x) = \hat{h}_o(x) \int_o^\infty dx_\lambda \omega_2(x_\lambda) z'(x_\lambda) R(x,x_\lambda) - \frac{z'(x)^2 \operatorname{sgn}(x) R(\infty,|x|)}{2}$$
$$- \operatorname{sgn}(x)\hat{h}_o(x) \cdot \int_o^{|x|} dx_\lambda R(\infty,x_\lambda)\omega_2(x_\lambda) z'(x_\lambda)$$

(3.99)

where $R(\infty,|x|)$ is the pseudofunction:

$$R(\infty, x) = \text{Pf.} \int_o^\infty dy/(z(y)-z(x))^2 \qquad (3.100)$$

Rewriting $g_2(x)$ in the form:

$$g_2(x) = \hat{h}_o(x) \int_o^\infty R(x,x_\lambda) z'(x_\lambda)\omega_2(x_\lambda)\, dx_\lambda$$
$$- \frac{1}{2}\frac{d}{dx}\left[z'(|x|) \int_o^{|x|} R(\infty,x_\lambda)\omega_2(x_\lambda) dx_\lambda \right]$$

(3.101)

and integrating, we obtain

$$\int_{-\infty}^{x} g_2(y)\, dy = \int_{-\infty}^{x} \hat{h}_o(y) \int_o^\infty dx_\lambda \omega_2(x_\lambda) z'(x_\lambda) R(y,x_\lambda)\, dy$$
$$+ \pi^{\frac{1}{2}}/2 \int_o^\infty dx_\lambda R(\infty,x_\lambda)\omega_2(x_\lambda) z'(x_\lambda)$$
$$- \frac{z'(|x|)}{2} \int_o^{|x|} dx_\lambda R(\infty,x_\lambda)\omega_2(x_\lambda) z'(x_\lambda)$$

(3.102)

In all these expressions we leave it implicit that the quantities R are pseudofunctions and that the taking of finite parts is carried out as necessary. The double integral above may well not be interchangeable. With a certain caution we may invert the order of integration in the crucial term. A sufficient condition for this to be possible and one adequate for present needs is that the function $\omega_2(x_\lambda)$ should satisfy a Lipschitz condition. In this way one can simplify as follows:

$$\int_{-\infty}^{x} d\hat{y}h_o(y) \int_0^{\infty} dx_\lambda \omega_2(x_\lambda) z'(x_\lambda) R(y,x_\lambda)$$

$$= \int_0^{\infty} dx_\lambda \omega_2(x_\lambda) z'(x_\lambda) \int_{-\infty}^{x} d\hat{y}h_o(y) R(y,x_\lambda)$$

$$= z'(x)/2 \int_0^{\infty} dy \omega_2(y) z'(y) R(x,y) - \pi^2/2 \int_0^{\infty} dy z'(y) \omega_2(y) R(\infty,y)$$

$$+ \quad \text{Pf.} \int_0^{\infty} dy \omega_2(y) z'(y) / (z(x)-z(y)) \qquad (3.103)$$

Putting this result back into (3.102), we arrive by further manipulations, not at an explicit expression for $\omega_2(\lambda)$ comparable to $\omega_1(\lambda)$ for the even case, but as an integral equation for the unknown function. This is, however, readily reduced to standard form, in fact to one of the Carleman type. (Hoare and Rahman 1974). The standardized equation reads

$$\frac{z'(x)^3 R(\infty,x) \omega_2(x)}{z''(x)} + \text{Pv.} \int_0^{\infty} \frac{dy \omega_2(y)}{(x-y)} = q_2(x) \qquad (3.104)$$

The Cauchy principal value (Pv.) appearing for the first time arises through the basic identity:

$$\text{Pv.}1/t = \text{Pf.}H(t)/t - \text{Pf.}H(-t)/t \qquad (3.104)$$

(Zemanian 1965). Let us define the function

$$q_2(x) = 2\int_{-\infty}^{x} g_2(y)dy - \frac{2z'(x)g_2(x)}{z''(x)} . \qquad (3.105)$$

By defining $\alpha(x) = \dfrac{z'(x)^3 R(\infty,x)}{z''(x)}$ (3.106)

the solution, in standard form, follows as

$$\omega_2(x) = \frac{\alpha(x)q_2(x)}{(\alpha^2+\pi^2)} + \frac{e^{\Delta(x)}}{(\alpha^2+\pi^2)^{\frac{1}{2}}}\,\text{Pv.}\int_0^{\infty}\frac{e^{-\Delta(y)}q_2(y)dy}{(\alpha^2+\pi^2).(x-y)}$$

where (3.107)

$$\Delta(x) = \pi^{-\frac{1}{2}}\text{Pv.}\int_0^{\infty}\frac{\Theta(\lambda)d\lambda}{(\lambda-\lambda_0(x))}$$

is the Hilbert transform of the function $\Theta(\lambda) = \underset{(o,\pi)}{\tan^{-1}}\pi/\alpha(\lambda)$.

The Carleman equation is treated rigorously by Muskhelishvili (1953). The existence of the above formal solution , under the assumptions mentioned above, is sufficient for present purposes to prove the completeness of the odd eigendistributions, for an implicitly defined class of generalised functions.

The method of Laplace transformation gives an

elegant proof of the completeness of the odd eigendistributions (see chapter four). If we accept that the above proof is valid, then the orthogonality property together with the Poincaré-Bertrand theorem can be used to find explicit expression for $b(\lambda)$. From (3.98) we have

$$\int_{-\infty}^{\infty} dx g_2(x)\phi_{od}(x,\lambda) = \int_{-\infty}^{\infty} dx \hat{h}_o(x)\phi_{od}(x,\lambda) . \int_{1}^{\infty} d\lambda' b(\lambda')\phi_{od}(x,\lambda') \qquad (3.108)$$

where from (3.80)

$$\phi_{od}(x,\lambda) = A_2(\lambda)(R(x,\lambda) - \alpha(x,\lambda)) \qquad (3.109)$$

where for convenience, we have defined

$$\alpha(x,\lambda) = R(\infty,\lambda).\Big[(H(x-|x_\lambda|)-H(-x-|x_\lambda|)) + R(\infty,\lambda)q(x_\lambda).(\delta(x-|x_\lambda|)-\delta(x+|x_\lambda|))\Big] \qquad (3.110)$$

($q(x) = z'(|x|)/z''(x)$).

If the order of integration could be exchanged in (3.108) then using the orthogonality integral I_2 (3.85) we would have

$$\int_{-\infty}^{\infty} dx g_2(x)\phi_{od}(x,\lambda) = A_2(\lambda)^2 N_2(\lambda) b(\lambda) \qquad (3.111)$$

From (3.108) we have

$$\int_{-\infty}^{\infty} dx g_2(x)\phi_{od}(x,\lambda) = \beta_3 + \int_{0}^{1} d\lambda' b(\lambda') A_2(\lambda) A_2(\lambda') \beta_4 \qquad (3.112a)$$

where

$$\beta_3 = \int_{-\infty}^{\infty} dx \hat{h}_0(x) A_2(\lambda) R(x,\lambda) \int_1^{\infty} d\lambda' A_2(\lambda') b(\lambda') R(x,\lambda') \qquad (3.112b)$$

and

$$\beta_4 = \int_{-\infty}^{\infty} dx \hat{h}_0(x) . (\alpha(x,\lambda)\alpha(x,\lambda') - \alpha(x,\lambda)R(x,\lambda') - \alpha(x,\lambda')R(x,\lambda)) \qquad (3.112c)$$

The order of integration in the second term on the left-hand side of (3.112c) has been exchanged but the order of integration in β_3 cannot be exchanged because it involves a product of two pseudofunctions $R(x,\lambda)$ and $R(x,\lambda')$. (see page 68 of the monograph by K.M.Case and P.F.Zweifel 1967.) In order to exchange the order of integration in β_3 we need a Poincaré-Bertrand type of formula for our pseudofunctions.

The pseudofunction $R(x,\lambda)$ can be written as

$$R(x,\lambda) = Pf. \int_0^{\infty} du / (z(u)-z(x_\lambda))^2$$

$$= R_{regular} + R_{singular} \qquad (3.113a)$$

where

$$R_{regular} = sgn(x) . \int_0^{|x|} du \left(\frac{1}{(z(u)-z(x_\lambda))^2} - \frac{1}{z'(x_\lambda)^2 (u-x_\lambda)^2} \right) \qquad (3.113b)$$

$$R_{singular} = \frac{-sgn(x)}{z'(x_\lambda)^2} Pf. \int_0^{|x|} \frac{du}{(u - x_\lambda)^2}$$

$$= \frac{+sgn(x)}{z'(x_\lambda)^2} Pv. \frac{1}{|x| - |x_\lambda|} + \frac{sgn(x)}{z'(x_\lambda)^2 . x_\lambda} \qquad (3.113c)$$

(see Appendix C for details). From above it can be seen that integration with $R(x,\lambda)$ as an integrand will involve ' Cauchy principal values '. Therefore, the only term where integrals cannot be exchanged is the term involving $R_{singular}$ component of $R(x,\lambda)$. In β_3 this will be the integral

$$I_7 = \int_{-\infty}^{*\infty} \frac{dx\,sgn(x)\hat{h}_o(x)A_2(x_\lambda)}{(|x|-|x_\lambda|)z'(x_\lambda)^2} \int_o^{*\infty} \frac{dx_{\lambda'}z'(x_{\lambda'})A_2(x_{\lambda'})sgn(x)}{(|x|-|x_{\lambda'}|)\,z'(x_{\lambda'})^2}$$

(3.114)

(We have used the notation * to show that the integral must be understood in the sense of principal values.)(Tricomi 1957) In order to exchange the order of integration in the above double integral, we note that the Poincaré-Bertrand theorem in its most general form states that: (Tricomi 1957)

$$\int^{*} \frac{dx}{x-x_\lambda} \int^{*} \frac{F(x_\lambda,x_{\lambda'},x)dx_{\lambda'}}{x_{\lambda'}-x} = \int^{*} dx_\lambda \int^{*} \frac{dx F(x_\lambda,x_{\lambda'},x)}{(x-x_\lambda)(x_{\lambda'}-x)} - \pi^2 F(x_\lambda,x_\lambda,x_\lambda)$$

(3.115)

Hence using the theorem,

$$I_7 = \int_o^{*\infty} \frac{dx}{(x-x_\lambda)} \int_o^{*\infty} dx_{\lambda'} \frac{A_2(\lambda)A_2(\lambda')b(\lambda')z''(x)}{-(x_{\lambda'}-x)\,z'(x_{\lambda'})z'(x_\lambda)^2}$$

$$= \int_o^{*\infty} dx_{\lambda'} \int_o^{*\infty} dx \frac{z''(x)A_2(\lambda)A_2(\lambda')b(\lambda')}{(x-x_\lambda).(x-x_{\lambda'}).\,z'(x_{\lambda'})z'(x_\lambda)^2} + D(\lambda)$$

(3.116)

where

$$D(\lambda) = \frac{\pi^2 b(\lambda) A_2(\lambda)^2 z''(x_\lambda)}{|z'(x_\lambda)|^3} \qquad (3.117)$$

It follows that when integrals are exchanged an extra term $D(\lambda)$ has to be added to the left hand-side of equation(3.108) and therefore,

$$\int_{-\infty}^{\infty} dx g_2(x) \phi_{od}(x,\lambda) = A_2(\lambda)^2 b(\lambda) . (N_2(\lambda) + \pi^2 z''(x_\lambda)/z'(|x_\lambda|)^3) \qquad (3.118)$$

If we define the normalized odd eigendistributions $\tilde{\phi}_{od}(x,\lambda)$ to be

$$\tilde{\phi}_{od}(x,\lambda) = N_3(\lambda)^{+\frac{1}{2}} (R(x,\lambda) - \alpha(x,\lambda)) . \hat{h}_o(x)^{1/2} \qquad (3.119a)$$

where

$$N_3(\lambda) = \frac{g(\infty,\lambda)}{(R(\infty,\lambda)^2 + \pi^2 g(\infty,\lambda)^2)} \qquad (3.119b)$$

$$g(x,\lambda) = g(\infty,\lambda) . [H(x-|x_\lambda|) - H(-x-|x_\lambda|) + q(\lambda) . (\delta(x-|x_\lambda|) - \delta(x+|x_\lambda|))] \qquad (3.119c)$$

$$g(\infty,\lambda) = z''(x_\lambda)/z'(|x_\lambda|)^3 \qquad (3.119d)$$

$$\alpha(x,\lambda) = \frac{R(\infty,\lambda) g(x,\lambda)}{g(\infty,\lambda)} \qquad (3.119e)$$

$$q(x_\lambda) = z'(|x_\lambda|)/z''(x_\lambda) \qquad (3.119f)$$

then

$$\int_{-\infty}^{\infty} dx\, \tilde{\Phi}_{od}(x,\lambda)\tilde{\Phi}_{od}(x,\lambda') = \delta(\lambda-\lambda') \qquad (3.120)$$

and

$$b(\lambda) = \int_{-\infty}^{\infty} dx g_2(x)\tilde{\Phi}_{od}(x,\lambda) \qquad (3.121)$$

The reason for introducing the function $g(x,\lambda)$ will become clear in the next chapter.

Section 3.7. Completeness and Vitali's Condition

The closure condition of Vitali (1921) (see Tricomi 1957 page 93) can be stated as follows:

" A necessary and sufficient condition for the completeness of an ON-system of L_2 - functions ($\phi_n(x)$) in the entire L_2 is that

$$\sum_n \left(\int_a^x \phi_n(y)dy \right)^2 = x-a \qquad (a<x<b) \text{ "}$$

Although the odd and even eigendistributions are not L_2 type being in fact distributions in the sense of Schwartz, in some cases the normalised versions of these functions can be treated as L_2-type of functions. In fact, seemingly strange relationships can be derived, which on a closer inspection prove to be quite simple. Below we present a simple proof that Vitali condition holds for both even and odd distributions.

Let $f(x,\lambda)$ denote either the normalised even

or the odd distributions. (It should be stated that the normalisation integral (3.120) is a symbolic realationship.) By expanding $\delta(q-x_o)$ it can be shown that

$$\delta(q-x_o) = \int_1^\infty d\lambda f(x_o,\lambda)f(q,\lambda) \qquad (3.122)$$

where the symbolic relationship is

$$\int_{-\infty}^{\infty} dx_o f(x_o,\lambda)f(x_o,\lambda') = \delta(\lambda-\lambda') \qquad (3.123)$$

Therefore,

$$\int_1^\infty d\lambda \left(\int_o^x f(x_o,\lambda)dx_o \right)^2 = \int_1^\infty d\lambda \int_o^x f(x,\lambda)dx \int_o^x f(q,\lambda)dq$$

$$= \int_o^x\int_o^x\int_1^\infty dxdqd\lambda f(x,\lambda)f(q,\lambda)$$

$$= \int_o^x\int_o^x dxdq\ \delta(x-q)$$

$$= (x-a) \qquad \text{Q.E.D.} \qquad (3.124)$$

For even distributions it can be proved by actual multiplication and integration that

$$1/\pi^{\frac{1}{2}}\left(\int_o^x \hat{h}_o(y)^{\frac{1}{2}}dy \right)^2 + \int_o^\infty d\lambda \left(\int_o^x \hat{\Phi}_{ev}(y,\lambda)dy \right)^2 = x$$

$$(3.125)$$

For the fundamental initial condition $P(x,o)=\delta(x-x_o)$ we can now immediately write

$$P(x,\tau) = \int_1^\infty d\lambda \tilde{\Phi}_{od}(x_o,\lambda)\check{\Phi}_{od}(x,\lambda)e^{-\lambda\tau} + \hat{h}_o(x)/\pi^{\frac{1}{2}}$$
$$+ \int_1^\infty d\lambda \hat{\Phi}_{ev}(x.\lambda)\hat{\Phi}_{ev}(x_o,\lambda)e^{-\lambda\tau} \qquad (3.126)$$

In chapter four, the above result is discussed in detail. If one could prove the above result for tau equal to zero then the completeness of both the even and odd distributions would be ascertained. The Laplace transformation method is used in the next chapter to prove this result.

CHAPTER FOUR

EXACT TRANSFORM SOLUTION OF THE SPECIAL MODEL

Section 4.1. Introduction

In this chapter, the full range initial value problem for velocity relaxation in one dimensional ensemble of Rayleigh test-particles is examined for the special Rayleigh model, using the Laplace transform method. The explicit solution in terms of two independent parity components is obtained. A connection has been made with the singular eigendistribution method of solving the initial value problem. The even component describes the speed relaxation and the odd component provides the time dependent flux of particles with the given velocity.

Bearing in mind the difficulties outlined in chapter three and the parallels between this situation and that encountered in other idealised problems in particle transport theory (Williams 1971) one is tempted to abandon the method of singular eigendistributions and revert to a more straightforward transform method. The result is an exact solution in the transform variable, which can easily be expressed in terms of integrals over known functions. Although the transform method is not encumbered with all the difficulties associated with the singular eigendistribution method, it is nevertheless, as we shall show, fundamentally equivalent to the method of singular eigendistributions.

The fact that these methods are identical,

follows quite logically if 'distributions' in the sense of Schwartz are defined as boundary values of analytic functions in the complex plane. (see e.g. Bremerman 1965.) Analytic representations of 'distributions' have been investigated by Köthe (1952), Tillman(1961), Sato(1959) and many others. These authors rely on techniques from functional analysis and topological vector spaces. The simplest discussion of this subject can be found in a monograph by H.Bremermann (1965). The following property plays a crucial role in the theory of representations of 'distributions' by analytic functions in the complex plane:

$$\text{Limit}_{\varepsilon \to 0_+} \left(f(x+i\varepsilon) - f(x-i\varepsilon) \right) = f(x) \quad \text{for all } x \qquad (4.1)$$

Thus, while it is impossible to represent f(x) as the restriction of an analytic function, any f(x) can be represented by a jump that f(s) makes as we pass from above the real axis to just below the real axis. Thus if T_d is a Schwartz distribution then there exists a function F(s) analytic everywhere except possibly on the real axis such that:

$$\text{Limit}_{\varepsilon \to 0_+} \int dx \phi(x) . \left(F(x+i\varepsilon) - F(x-i\varepsilon) \right) = \langle T_d, \phi(x) \rangle \qquad (4.2)$$

for any test function $\phi(x)$ of class D . F(s) is called the analytic representation of T_d.

Recasting equation in the scaled variables x, and with the usual definitions given in chapter three, we have (see (3.4) and (3.7))

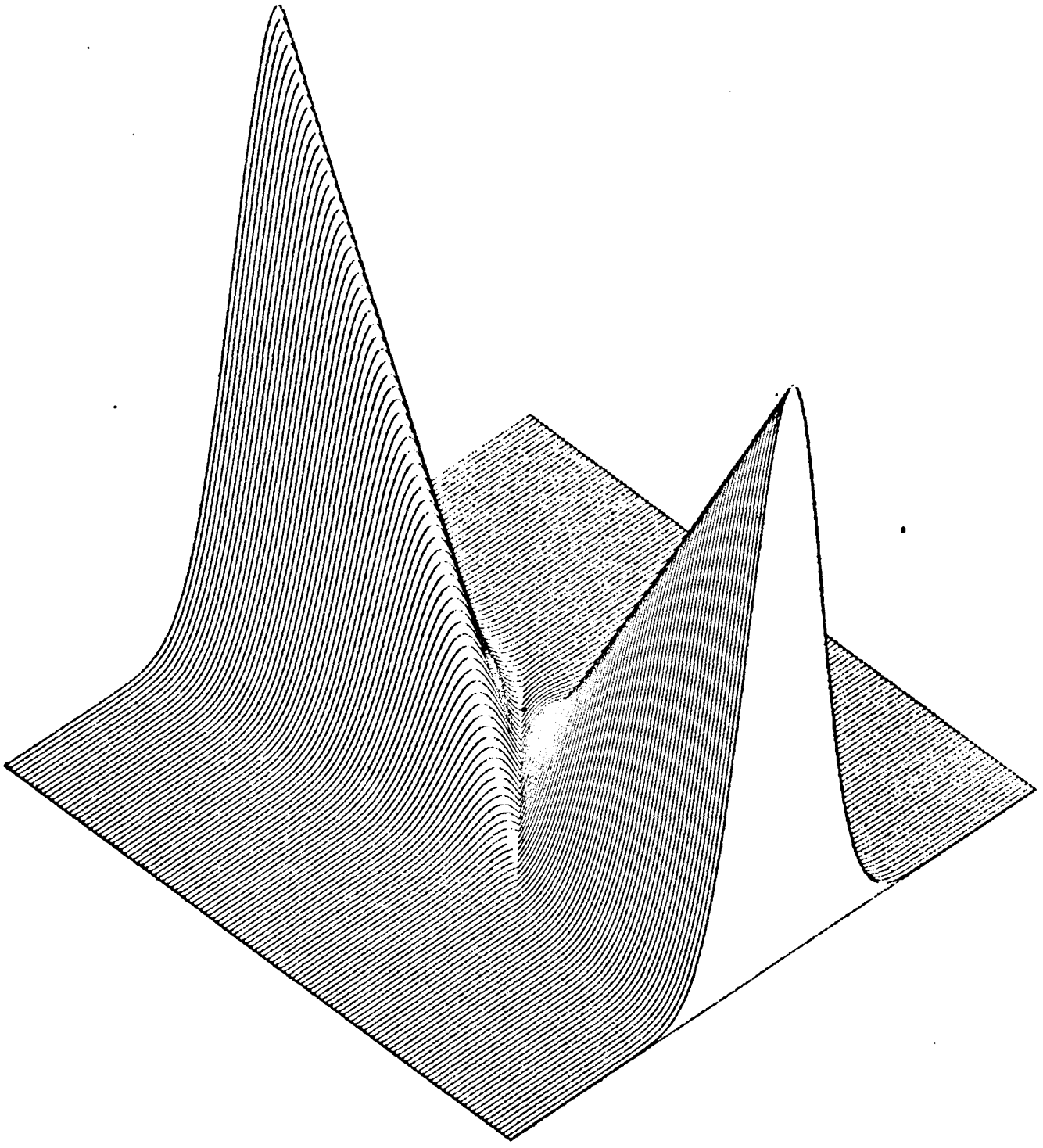


Figure 8: The Rayleigh Kernel K(x|y) for unit mass ratio and Maxwellian heat-bath. The vertical scale is arbitrary, the x and y intervals plotted from -10 to +10 with the origin at the centre. Note the discontinuity of the first derivative visible along the diagonal.

$$\frac{\partial P_{ev}(x,\tau)}{\partial \tau} = 2\hat{h}_o(x)\int_o^\infty dy\ \max(|x|,y)P_{ev}(y,\tau) - z(x)P_{ev}(x,\tau)$$

(4.3a)

$$\frac{\partial P_{od}(x,\tau)}{\partial \tau} = -2\mathrm{sgn}(x)\hat{h}_o(x)\int_o^\infty dy \min(|x|,y)P_{od}(y,\tau) - z(x)P_{od}(x,\tau)$$

(4.3b)

Although it is possible to work with the uncoupled equation (3.7) and arbitrary initial condition $P(x,o)$, it has proved to be more convenient to work with the fundamental initial condition $P(x,o) = \delta(x-x_o)$ and the above pair of equations.(see Barker et al 1977 for the alternative approach) By using the superposition principle one can always find the solution for arbitrary initial condition $P(x,o)$ once the solution for the fundamental initial condition is known.

In the next section, the method of Laplace transform is applied successively to (4.3a) and (4.3b) with $P(x,o) = \delta(x-x_o)$

Section 4.2. The Laplace Transform Solution

(a) Even Solution

By making a further change of the dependent variable

$$P(x,\tau) = \hat{h}_o(x)f_{ev}(x,\tau) \qquad (4.4)$$

the even component of the transport equation becomes

$$\frac{\partial f_{ev}(x,\tau)}{\partial \tau} = 2\int_0^\infty dy \max(|x|,y)\hat{h}_o(y)f_{ev}(y,\tau) - z(x)f_{ev}(x,\tau) \qquad (4.5)$$

with the initial conditions:

$$P_{ev}(x,o) = \frac{1}{2}.(\ \delta(x-x_o)+\delta(x+x_o)\ ) \qquad (4.6)$$

$$f_{ev}(x,\tau) = P_{ev}(x,o)/\hat{h}_o(x)$$

The Laplace transform can be defined compactly in operator form as

$$\hat{L}f_{ev}(x,\tau) = f_{ev}(x,s)$$

$$= \int_0^\infty d\tau \exp(-s\tau) f_{ev}(x,\tau) \qquad (4.7)$$

and the inverse transform as

$$\hat{L}^{-1}f_{ev}(x,s) = \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds \exp(s\tau) f_{ev}(x,s)$$

$$\sigma > o$$

$$= f_{ev}(x,\tau) \qquad (4.8)$$

Applying the transform operator to (4.5) one obtains

$$(\ z(x)+s\ )f_{ev}(x,s) - 2\int_0^\infty dy \max(|x|,y)h_o(y)f_{ev}(y,s) = f_{ev}(x,o)$$

$$(4.9)$$

To show that the above integral equation can be solved

exactly, it is convenient to reduce it first to a differential equation. Differentiating with respect to x twice and making use of the identity

$$\frac{d^2}{dx^2}|x-y| = 2\delta(x-y) \qquad (4.10)$$

one finds after some rearrangements and simplifications

$$f''_{ev}(x,s) + 2z'(x)f'_{ev}(x,s)/(z(x)+s) = \frac{P''_{ev}(x,o)}{\hat{h}_o(x_o)(z(x)+s)} \qquad (4.11)$$

The primes indicating differentiation with respect to x. The classical solution of equation (4.11) is given by

$$U(x,s) = A(s)/(z(x)+s)^2 \qquad (4.12)$$

where A(s) is function of s only. The general solution of (4.11) follows as

$$f'_{ev}(x,s) = U(x,s)V(x,s) \qquad (4.13)$$

where

$$V'(x,s) = \frac{1}{U(x,s)} \cdot \left\{ \frac{P''_{ev}(x,o)}{\hat{h}_o(x_o)(z(x)+s)} \right\} \qquad (4.14)$$

where having found $f'_{ev}(x,s)$ we shall integrate it to obtain $f_{ev}(x,s)$. In order to find $V(x,s)$ one requires the following identities:

$$(z(x)+s)P'_{ev}(x,o) = (z(x_o)+s)P'_{ev}(x,o) - |z'(x_o)| P_{od}(x,o) \qquad (4.15)$$

where

$$P_{od}(x,o) = \frac{\delta(x-x_o)-\delta(x+x_o)}{2} \qquad (4.16)$$

and

$$(z(x)+s)P''_{ev}(x,o) = (z(x_o)+s)P''_{ev}(x,o) - 2|z'(x_o)| P'_{od}(x,o) + 2\hat{h}_o(x_o)P_{ev}(x,o) \qquad (4.17)$$

Therefore,

$$V'(x,s) = \frac{1}{A(s)h_o(x_o)} \left[(z(x_o)+s)P''_{ev}(x,o) - 2|z'(x_o)| P'_{od}(x,o) + 2\hat{h}_o(x_o)P_{ev}(x,o) \right] \qquad (4.18)$$

In this form $V'(x,s)$ can easily be integrated to give

$$V(x,s) = \frac{1}{A(s)} \left[\frac{(z(x_o)+s)P'_{ev}(x,o)}{\hat{h}_o(x_o)} - \frac{2\, z'(x_o)P'_{od}(x,o)}{\hat{h}_o(x_o)} + (H(x-x_o)+H(x+x_o)) \right] + B(s) \qquad (4.19)$$

where $B(s)$ is a constant of integration.

Therefore,

$$f'_{ev}(x,s) = \frac{(z(x_o)+s)P'_{ev}(x,o)}{(z(x)+s)^2\hat{h}_o(x_o)} - \frac{2|z'(x_o)|P_{od}(x,o)}{(z(x)+s)^2\hat{h}_o(x_o)}$$

$$+ \frac{H(x-x_o)+H(x+x_o)}{(z(x)+s)^2} + \frac{C(s)}{(z(x)+s)^2} \qquad (4.20)$$

where $C(s) = A(s)B(s)$. However, $C(s)$ must be zero because $f'_{ev}(x,s)$ is an odd function of x and $(z(x)+s)$ is even function of x.

In order to integrate $f'_{ev}(x,s)$, the following identity is required:

$$\frac{P'_{ev}(x,o)}{(z(x)+s)^2} = \frac{P'_{ev}(x,o)}{(z(x_o)+s)^2} + \frac{2|z'(x_o)|P_{od}(x,o)}{(z(x_o)+s)^3} \qquad (4.21)$$

which simplifies $f'_{ev}(x,s)$ to give

$$f'_{ev}(x,s) = \frac{P'_{ev}(x,o)}{(z(x_o)+s)\hat{h}_o(x_o)} + \frac{H(x-x_o)+H(x+x_o)}{(z(x)+s)^2} \qquad (4.22)$$

Simple integration gives

$$f_{ev}(x,s) = \frac{P_{ev}(x,o)}{(z(x_o)+s)\hat{h}_o(x_o)} - \int_{\max(|x|,|x_o|)}^{\infty} \frac{du}{(z(u)+s)^2} + D(s) \qquad (4.23)$$

where D(s) is a constant of integration. D(s) is found by substituting $f_{ev}(x,s)$ from above into (4.9). For this substitution the following integral is required:

$$2\int_0^\infty dy \max(|x|,y)\hat{h}(y)\int_{\max(|x|,|x_o|)}^\infty dt/(z(t)+s)^2 = \frac{\max(|x|,|x_o|)}{(z(x_o)+s)} + (z(x)+s)\int_{\max(|x|,|x_o|)}^\infty dt/(z(t)+s)^2 - 1/\pi^{\frac{1}{2}} \qquad (4.24)$$

After the substitution D(s) is found to be

$$D(s) = 1/s\pi^{\frac{1}{2}} \qquad (4.25)$$

Therefore,

$$P_{ev}(x,s) = \frac{\hat{h}_o(x)}{\pi^{\frac{1}{2}}s} - \hat{h}_o(x)\int_{\max(|x|,|x_o|)}^\infty dt/(z(t)+s)^2 + \frac{P_{ev}(x,o)}{(z(x)+s)} \qquad (4.26)$$

where

$$\hat{L}P_{ev}(x,\tau) = P_{ev}(x,s) \qquad (4.27)$$

By applying the operator $\hat{L}^{-1}$ to (4.26) one obtains

$$P_{ev}(x,\tau) = P_{ev}(x,o)\exp(-z(x)\tau) + \hat{h}_o(x)/\pi^{\frac{1}{2}} - \tau\hat{h}_o(x)\int_{\max(|x|,|x_o|)}^\infty du\, e^{-z(u)\tau} \qquad (4.28)$$

where the relationship:

$$\hat{L}^{-1}\int_0^x du/(z(u)+s)^2 = \tau\int_0^x du\exp(-z(u)\tau) \qquad (4.29)$$

has been used. This follows quite simply if the order of integration on the left hand-side of (4.29) is exchanged. In Appendix D this relationship is proved rigorously.

(b) Odd Solution

By making a further change of the the dependent variable

$$P_{od}(x,\tau) = \hat{h}_o(x) f_{od}(x,\tau) \qquad (4.30)$$

the odd component of the transport equation becomes

$$\frac{\delta f_{od}(x,\tau)}{\delta \tau} = -2\mathrm{sgn}(x)\int_0^\infty dy \min(|x|,y)\hat{h}_o(y) f_{od}(y,\tau) - z(x) f_{od}(x,\tau) \qquad (4.31)$$

with the initial conditions:

$$P_{od}(x,o) = \frac{\delta(x-x_o)-\delta(x+x_o)}{2} \qquad (4.32)$$

$$f_{od}(x,o) = \frac{P_{od}(x,o)}{\hat{h}_o(x_o)} \qquad (4.33)$$

By applying the operator $\hat{L}$ to (4.31) one obtains

$$(z(x)+s)f_{od}(x,s) + 2\mathrm{sgn}(x) \int_0^{\infty} dy \min(|x|,y)\hat{h}_o(y)f_{od}(y,s) = f_{od}(x,o) \qquad (4.34)$$

By differentiating twice, as in the case of the even solutions above (see (a) above), and after some rearrangements and simplifications, one finds that

$$f''_{od}(x,s) + \frac{2z'(x)f'_{od}(x,s)}{(z(x)+s)} = \frac{P''_{od}(x,o)}{\hat{h}_o(x_o).(z(x)+s)} \qquad (4.35)$$

From the general theory the solution of this equation is given by

$$f'_{od}(x,s) = U(x,s).V(x,s) \qquad (4.36)$$

where the classical solution as in the case of the even component is

$$U(x,s) = \frac{A(s)}{(z(x)+s)^2} \qquad (4.37)$$

and

$$V'(x,s) = \frac{P''_{od}(x,o)}{U(x,s)\hat{h}_o(x_o).(z(x)+s)} \qquad (4.38)$$

In order to integrate (4.38) one requires the following identities:

$$(z(x)+s)P'_{od}(x,o) = (z(x_o)+s)P'_{od}(x,o) - |z'(x_o)| P_{ev}(x,o)$$

(4.39a)

and

$$(z(x)+s)P''_{od}(x,o) = (z(x_o)+s)P''_{od}(x,o) - 2|z'(x_o)| P'_{ev}(x,o) + 2\hat{h}_o(x_o)P_{od}(x,o)$$

(4.39b)

By substituting in (4.38) and integrating we have

$$V(x,s) = \frac{(z(x_o)+s) P'_{od}(x,o)}{A(s)\hat{h}_o(x_o)} - \frac{2|z'(x_o)| P_{ev}(x,o)}{A(s)\hat{h}_o(x_o)} + \frac{H(x-x_o)-H(x+x_o)}{A(s)} + B(s)$$

(4.40)

B(s) is a constant of integration.

Therefore,

$$f'_{od}(x,s) = \frac{(z(x_o)+s)P'_{od}(x,o)}{(z(x)+s)^2\hat{h}_o(x_o)} - \frac{2|z'(x_o)| P_{ev}(x,o)}{(z(x)+s)^2\hat{h}_o(x_o)} + \frac{H(x-x_o)-H(x+x_o)}{(z(x)+s)^2} + \frac{C(s)}{(z(x)+s)^2}$$

(4.41)

where $C(s) = B(s).A(s)$.

By using the identity

$$\frac{P'_{od}(x,o)}{(\,z(x)+s\,)^2} = \frac{P'_{od}(x,o)}{(\,z(x_o)+s)^2} + \frac{2|z'(x_o)|\;P_{ev}(x,o)}{(\,z(x_o)+s\,)^3} \qquad (\,4.42\,)$$

we can re-write (4.41) in the form:

$$f'_{od}(x,s) = \frac{P'_{od}(x,o)}{(\,z(x_o)+s)\hat{h}_o(x_o)} + \frac{H(x-x_o)-H(x+x_o)}{(\,z(x)+s\,)^2} + \frac{C(s)}{(\,z(x)+s\,)^2} \qquad (\,4.43\,)$$

This equation can easily be integrated to give

$$f_{od}(x,s) = \frac{P_{od}(x,o)}{(\,z(x_o)+s)\hat{h}_o(x_o)} - \mathrm{sgn}(x)\mathrm{sgn}(x_o)\int_o^{\min(|x|,|x_o|)} \frac{du}{(z(u)+s)^2} + C(s)\int_o^x \frac{du}{(z(u)+s)^2} + D(s) \qquad (\,4.44\,)$$

$D(s)$ is a constant of integration which must be zero because $f_{od}(x,s)$ is an odd function of x.

In order to find $C(s)$, $f_{od}(x,s)$ from above is substituted in equation (4.34). By using the following

integrals

$$2\mathrm{sgn}(x)\mathrm{sgn}(x_o)\int_o^{\infty} dy \min(|x|,y)\hat{h}_o(y)\int_o^{\min(|x|,|x_o|)} du/(\,z(u)+s\,)^2$$

$$= -(\,z(x)+s\,)\mathrm{sgn}(x)\mathrm{sgn}(x_o)\int_o^{\min(|x|,|x_o|)} du/(\,z(u)+s\,)^2$$

$$+ \frac{\min(|x|,|x_o|)\mathrm{sgn}(x)\mathrm{sgn}(x_o)}{(\,z(x_o)+s\,)}$$

$$+ \pi^{\frac{1}{2}}x\int_o^{x_o} du/(\,z(u)+s\,)^2 \qquad (4.45)$$

and

$$2\mathrm{sgn}(x)\int_o^{\infty} dy \min(|x|,y)\hat{h}_o(y)\int_o^{y}\frac{du}{(\,z(u)+s\,)^2}$$

$$= -(\,z(x)+s\,)\int_o^{x}\frac{du}{(\,z(u)+s\,)^2} + x\pi^{\frac{1}{2}}\int_o^{\infty}\frac{du}{(\,z(u)+s\,)^2} \qquad (4.46)$$

C(s) is found to be

$$C(s) = \frac{Q(x_o,s)}{Q(\infty,s)} \qquad (4.47)$$

where by definition:

$$Q(x,s) = \int_o^{x}\frac{du}{(\,z(u)+s\,)^2} \qquad (4.48)$$

We have used the property $\pi^{\frac{1}{2}} = z'(\infty)$ in the above integrals.(see (3.13).) By substituting the value of C(s) in (4.44) we obtain

$$f_{od}(x,s) = \frac{P_{od}(x,o)}{\hat{h}_o(x_o)\,(\,z(x_o)+s)} - \mathrm{sgn}(x)\mathrm{sgn}(x_o)\int_o^{\min(|x|,|x_o|)} \frac{du}{(z(u)+s)^2}$$

$$+ \frac{Q(x_o,s)Q(x,s)}{Q(\infty,s)} \qquad (\ 4.49\ )$$

By applying the operator $\hat{L}^{-1}$ to $\hat{h}_o(x)f_{od}(x,s)$ one finds that

$$P_{od}(x,\tau) = P_{od}(x,o)\exp(-z(x_o)\tau)$$

$$- \tau\,\mathrm{sgn}(x)\mathrm{sgn}(x_o)\hat{h}_o(x)\int_o^{\min(|x|,|x_o|)} du\exp(-z(u)\tau)$$

$$+ \hat{h}_o(x)\ \hat{L}^{-1}\ \frac{Q(x_o,s)Q(x,s)}{Q(\infty,s)}$$

$$(\ 4.50\ )$$

There are many physically interesting results which can be obtained by using the above equation without actually finding the expression for the inverse of the complicated product on the right-hand side (Barker et al 1977). In the next section, the expession for the inverse is calculated in order to

establish a connection with our previous result in terms of pseudofunctions.

Section 4.3. Inverse Transform of the Product

For convenience let

$$B(x,x_o,s) = \frac{Q(x_o,s)Q(x,s)}{Q(\infty,s)} \qquad (4.51)$$

The existence of the inverse $\hat{L}^{-1}\, B(x,x_o,s)$ in equation (4.50) must be substantiated before one can find the expression for it. For this we need to show that the function $B(x,x_o,s)$ is of the order $O(s^{-k})$ with $k>1$, and analytic everywhere except along the branch-cut extending from minus one to minus infinity along the real line in the complex plane (see e.g. Churchill 1958). The analyticity condition is clearly fulfilled since the terms in the integrand are singular only on the branch-cut $Re(s) \leqslant -1$. To obtain the order in s, we use the bound—to-the-collision number function:

$$1 \leqslant z(x) \leqslant 1+\pi^{\frac{1}{2}}\, x\ ,$$

in view of which

$$|Q(x,s)| \ll |x|/|(s+1)^2| \qquad (4.52)$$

$$|Q(\infty,s)| > \left| \int_0^\infty \frac{dy}{(1+s+\pi^{\frac{1}{2}}y)^2} \right| = \frac{1}{\pi^{\frac{1}{2}}\,|s+1|} \qquad (4.53)$$

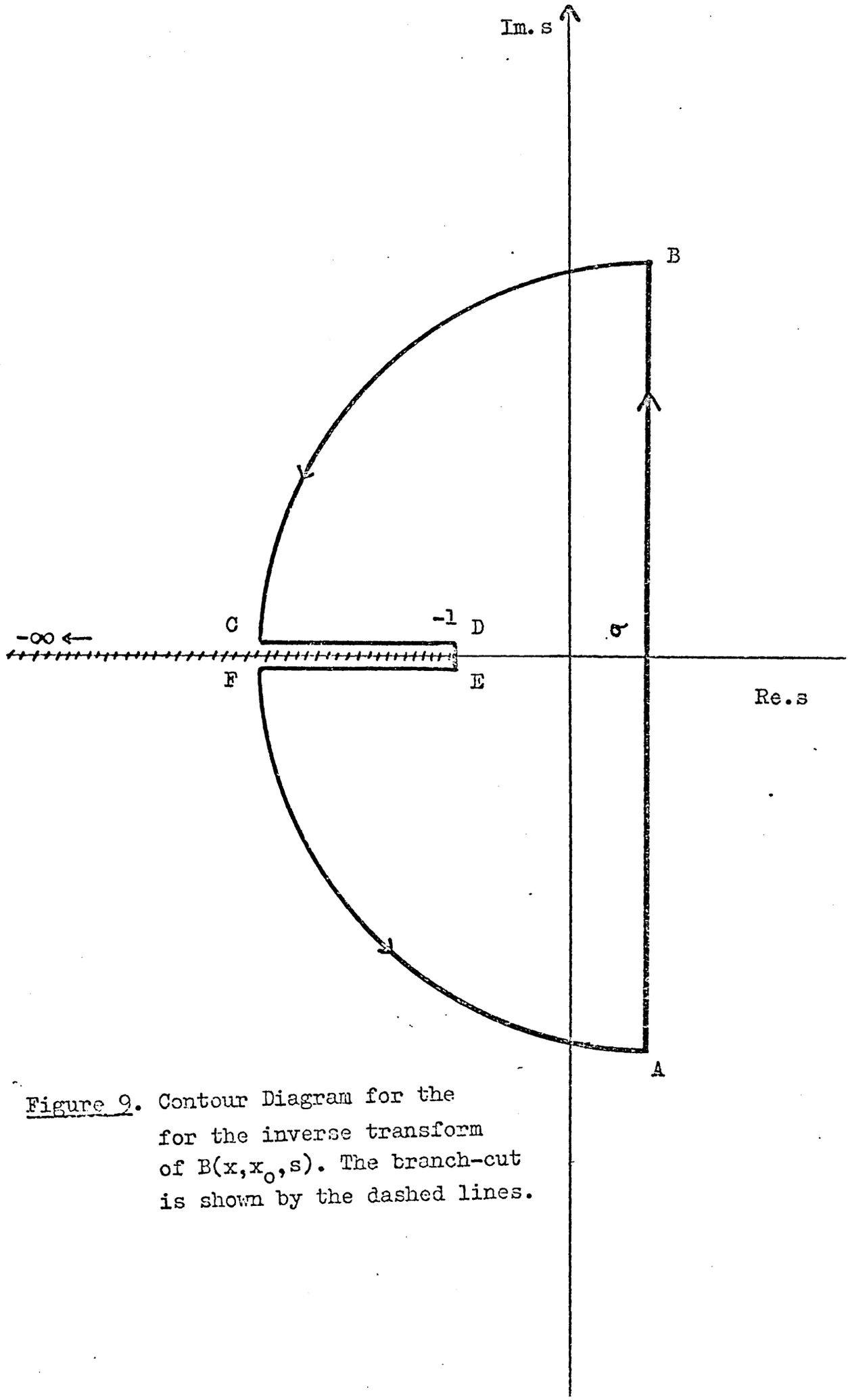


Figure 9. Contour Diagram for the for the inverse transform of $B(x,x_o,s)$. The branch-cut is shown by the dashed lines.

From this it follows immediately that

$$B(x,x_o,s) \ll \frac{|x.x_o|}{\pi^{\frac{1}{2}}|s+1|^{\frac{3}{2}}} \qquad (4.54)$$

and the existence of a well defined inverse is assured. The contour-diagram for finding the inverse transform of $B(x,x_o,s)$ is shown in figure 9 . From the diagram (see Appendix D) one can immediately write:

$$L^{-1}\, B(x,x_o,s) = \frac{1}{2\pi i} \int_1^{\infty} d\lambda\, e^{-\lambda\tau}\left(B^-(\lambda) - B^+(\lambda) \right)$$

where

$$B^-(\lambda) - B^+(\lambda) = \lim_{\varepsilon \to 0} \left(B(x,x_o,-\lambda-i\varepsilon) - B(x,x_o,-\lambda+i\varepsilon) \right)$$

$$= 2i \lim_{\varepsilon \to 0} \left(\mathrm{Im}\, B(x,x_o,-\lambda-i\varepsilon) \right) \qquad (4.55)$$

In Appendix D the following identity is derived

$$\lim_{\varepsilon \to 0} Q(x,-\lambda \pm i\varepsilon) = R(x,\lambda) \pm i\pi g(x,\lambda) \qquad (4.56)$$

where $R(x,\lambda)$ is the pseudofunction defined by (3.75) and $g(x,\lambda)$ is defined by (3.119c):

$$g(x,\lambda) = g(\infty,\lambda).\Big[H(x-|x_\lambda|) - H(-x-|x_\lambda|) + q(\lambda).\left(\delta(x-|x_\lambda|) - \delta(x+|x_\lambda|) \right)\Big] \qquad (4.57a)$$

where

$$g(\infty,\lambda) = \frac{z''(x_\lambda)}{|z'(x_\lambda)|^3} \qquad (4.57b)$$

and

$$q(\lambda) = \frac{|z'(x_\lambda)|}{z''(x_\lambda)} \qquad (4.57c)$$

By simple multiplication

$$B(x,x_o,-\lambda-i\varepsilon) = \frac{Q(x,-\lambda-i\varepsilon)Q(x_o,-\lambda-i\varepsilon)Q(\infty,-\lambda+i\varepsilon)}{Q(\infty,-\lambda-i\varepsilon)Q(\infty,-\lambda+i\varepsilon)} \qquad (4.58)$$

By using the identity (4.56) we have

$$2i(\ \mathrm{Im}\ B^{-}(\lambda)\ ) = 2\pi i\ E(x,x_o,\lambda) \qquad (4.59)$$

where

$$E(x,x_o,\lambda) = \frac{g(\infty,\lambda)}{A(\lambda)}\cdot\left[R(x,\lambda)R(x_o,\lambda) - \pi^2 g(x_o,\lambda)g(x,\lambda)\right] - \frac{R(\infty,\lambda)}{A(\lambda)}\cdot\left[R(x,\lambda)g(x_o,\lambda) + R(x_o,\lambda)g(x,\lambda)\right] \qquad (4.60a)$$

where by definition

$$A(\lambda) = R(\infty,\lambda)^2 + \pi^2 g(\infty,\lambda)^2 \qquad (4.60b)$$

Therefore,

$$\hat{L}^{-1}\ B(x,x_o,s) = \int_o^\infty dx_\lambda z'(x_\lambda)E(x,x_o,\lambda)\exp(-z(x_\lambda)\tau) \qquad (4.61)$$

where the substitution $\lambda = z(x_\lambda)$ is implicit.

In order to write $\hat{L}^{-1} B(x,x_o,s)$ in a more intelligable form we recall that the odd orthonormalised eigendistributions were defined as (see (3.119)):

$$\tilde{\Phi}_{od}(x,\lambda) = N_3(\lambda)^{+\frac{1}{2}}(R(x,\lambda) - \alpha(x,\lambda)). \hat{h}_o(x)^{\frac{1}{2}} \qquad (4.62a)$$

where

$$N_3(\lambda) = \frac{g(\infty,\lambda)}{R(\infty,\lambda)^2 + \pi^2 g(\infty,\lambda)^2} \qquad (4.62b)$$

and

$$\alpha(x,\lambda) = \frac{R(\infty,\lambda)g(x,\lambda)}{g(\infty,\lambda)} \qquad (4.62c)$$

By simple multiplication it can be shown that

$$E(x,x_o,s) = \frac{\tilde{\Phi}_{od}(x_o,\lambda)\tilde{\Phi}_{od}(x,\lambda)}{\hat{h}_o(x)} - \frac{g(x_o,\lambda)g(x,\lambda)}{g(\infty,\lambda)} \qquad (4.63)$$

Therefore,

$$\hat{h}_o(x)\hat{L}^{-1} B(x,x_o,s) = \int_o^\infty dx_\lambda z'(x_\lambda) e^{-z(x_\lambda)\tau} \tilde{\Phi}_{od}(x_o,\lambda)\tilde{\Phi}_{od}(x,\lambda)$$

$$- \hat{h}_o(x) \int_o^\infty dx_\lambda z'(x_\lambda) e^{-z(x_\lambda)\tau} \frac{g(x_o,\lambda)g(x,\lambda)}{g(\infty,\lambda)} \qquad (4.64)$$

In Appendix D it is proved that:

$$\int_0^{\infty} dx_\lambda z'(x_\lambda) e^{-z(x_\lambda)\tau} \frac{g(x_o,\lambda)g(x,\lambda)}{g(\infty,\lambda)} = \frac{P_{od}(x,o)\ e^{-z(x_o)\tau}}{\hat{h}_o(x)}$$

$$- \operatorname{sgn}(x_o)\operatorname{sgn}(x)\tau \int_0^{\min(|x|,|x_o|)} du \exp(-z(u)\tau)$$

(4.65)

Section 4.4. The Complete Solution

By substituting the expression for $\hat{L}^{-1} B(x,x_o,s)$ (4.64) in equation (4.50) and using (4.65) it follows immediately that:

$$P_{od}(x,\tau) = \int_0^{\infty} dx_\lambda z'(x_\lambda) \exp(-z(x_\lambda)\tau)\ \tilde{\Phi}_{od}(x_o,\lambda)\tilde{\Phi}_{od}(x,\lambda)$$

(4.66)

This result connects the Laplace transform solution with the result obtained in chapter three by the method of singular eigendistributions. (see (3.126).) The solution in the above form self-evidently proves the completeness of the odd eigendistributions.

Similarly by direct multiplication it is relatively easy to prove that (see (4.28).)

$$P_{ev}(x,\tau) = \hat{h}_o(x)/\pi^{\frac{1}{2}} + \int_0^{\infty} dx_\lambda z'(x_\lambda) e^{-z(x_\lambda)\tau} \tilde{\Phi}_{ev}(x_o,\lambda)\tilde{\Phi}_{ev}(x,\lambda)$$

$$= P_{ev}(x,o)\exp(-z(x_o)\tau) + \hat{h}_o(x)/\pi - \hat{h}_o(x)\tau\int_{\max(|x|,|x_o|)}^{\infty} du\, e^{-z(u)\tau}$$

where from (3.96) (4.67)

$$\Phi_{ev}(x,\lambda) = g(\omega,\lambda)\,\big[H(x-x_\lambda)-H(x+x_\lambda) - q(\lambda).(\delta(x-|x_\lambda|)-\delta(x+|x_\lambda|))\big].$$

(4.68)

The complete solution can now immediately be written

$$P(x,\tau) = \delta(x-x_o)e^{-z(x_o)\tau} + \hat{h}_o(x)/\pi^{\frac{1}{2}} - \hat{h}_o(x)\tau\int_{\max(|x|,|x_o|)}^{\infty} du\, e^{-z(u)\tau} - \operatorname{sgn}(x_o)\operatorname{sgn}(x)\hat{h}_o(x)\int_{o}^{\min(|x|,|x_o|)} du\, e^{-z(u)\tau} + \hat{h}_o(x)\hat{L}^{-1}\,B(x,x_o,s) \qquad (4.69)$$

For arbitrary initial-condition $P(x,o)$, by the principle of superposition, the solution follows in the form:

$$P(x,\tau) = \int_{-\infty}^{\infty} dx_o\, P(x_o,o)P(x,x_o,\tau) \qquad (4.70)$$

where $P(x,x_o,\tau)$ is the solution (4.69) with the delta initial condition. More explicitly on integration the solution follows in the form:

$$P(x,\tau) = \underset{\text{(mixed)}}{P(x,o)\exp(-z(x)\tau)} + \underset{\text{(even)}}{\hat{h}_o(x)/\pi^{\frac{1}{2}}}$$

$$- 2\tau\hat{h}_o(x)/\pi^{\frac{1}{2}}\Big[\int_x^{\infty} e^{-z(u)\tau}\int_o^{u} \underset{\text{(even)}}{P_{ev}(v,o)}dv\,du$$

$$+ \int_o^{x} e^{-z(u)}\int_u^{\infty} \underset{\text{(odd)}}{P_{od}(v,o)}dv\,du\Big]$$

$$+ 2\hat{h}_o(x)\hat{L}^{-1}\left\{\frac{Q(x,s)}{Q(\infty,s)}\int_o^{\infty} \underset{\text{(odd)}}{P_{od}(v,o)}Q(v,s)dv\right\} \qquad (4.71)$$

In the next chapter, the complete solution is used to obtain physical properties of the model.

The numerical inverse of Laplace transform is nowadays quite straightforward and a number of excellent alogrithms are available. Although as we have showed, the inverse integral can be found, in practice, it turns out to be more advantageous to apply the straight numerical method of finding the inverse transform when pseudofunctions are involved. We were thus able to calculate the inverse $L^{-1}\,B(x,x_o,s)$ to an accuracy quite sufficient for illustrating the behaviour of the solutions under various initial-conditions. The method we employed was the Dubner-Abate (1968) procedure as improved by Dubin and Crump (1974) (see Figure 11). For numerical calculations, we have considered the delta initial condition and the Maxwellian heat-bath $\hat{h}_o(x) = \exp(-x^2)$.

Section 4.5. Barrier Problem by the Laplace Transform method

In past literature, the barrier problems were studied for systems where the interactions with a heat-bath can be specified in terms of mean collision number and the relaxation process can be considered in terms of discrete 'relaxation - times'(see e.g. Montroll and Shuler 1958). In these studies particular attention is paid to the dependence of overall rate of reaction (absorption) upon both the barrier energy and the initial distribution of reactant particles. A notable feature of all models so far treated is the existence of a characteristic first-order rate constant, with exponential dependence on barrier height (the Arrhenius law .) which can only be justified asymptotically for limitingly high barrier energy.

For the singular kinetic process describing the special Rayleigh model with absorption barrier, Hoare and Rahman (1976), probably for the first time, presented an exact solution. These authors used the method of singular eigenfunctions with the associated difficulties. Below the problem is solved by applying the transform method which again illustrates the simplicity and elegance of the method.

The transport equation for 'absorbing barrier' problem in the speed variable can immediately be written down if one identifies $2P_{ev}(x,\tau)$ with $P(|x|,\tau)$:

$$\frac{\partial P_{ev}(x,x^+,\tau)}{\partial \tau} = \hat{2h}_o(x) \int_o^\infty dy \max(x,y) P_{ev}(y,x^+,\tau)$$

$$- z(x) P_{ev}(x,x^+,\tau)$$

$$o < x_o < x^+ \qquad (4.72)$$

From above it is apparent that particles exceeding the speed-barrier x^+ would be removed from the system. In order to find $P_{ev}(x,x^+,\tau)$, we have to repeat all the steps taken to find the even parity solution. Working with the fundamental initial-condition $\delta(x-x_o)$ and making all the transformations it can be shown that:

$$f_{ev}(x,x^+,s) = \frac{P_{ev}(x,x^+,o)}{(z(x_o)+s)\hat{h}_o(x_o)} - \int_{\max(|x|,|x_o|)}^{x^+} \frac{du}{(z(u)+s)^2} + D(s)$$

$$o < x < x^+ \qquad (4.73)$$

After the relevant substitution D(s) is found to be

$$D(s) = \frac{1}{Z'(x^+)} \left[\frac{1}{(s + z(x^+) - x^+ z'(x^+))} \right.$$

$$\left. - \frac{1}{(z(x^+) + s)} \right] \qquad (4.74)$$

which finally leads to the solution:

$$P_{ev}(x,x^+,\tau) = P_{ev}(x,x^+,o)\exp(-z(x_o)\tau) - \hat{h}_o(x)\tau\int_{\max(|x|,|x_o|)}^{x^+} du\ e^{-z(u)\tau}$$

$$+ \frac{\hat{h}_o(x)}{z'(x^+)}\left[\exp(-z(x^+)\tau)\exp(-x^+z'(x^+)\tau) - \exp(-z(x^+)\tau)\right]$$

(4.75)

For the Maxwellian heat-bath we have

$$P(x,x^+,\tau) = \frac{2e^{-x^2}}{z'(x^+)}\left(\exp(-e^{-x^{+2}}\tau) - \exp(-z(x^+)\tau)\right)$$

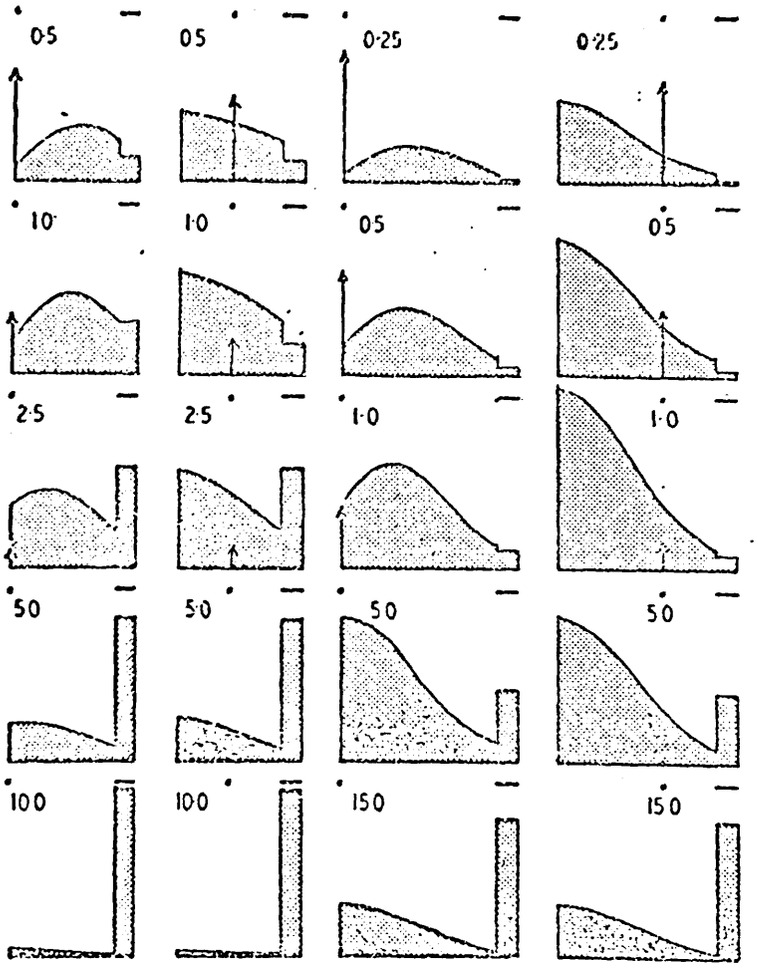
$$+ \delta(x-x_o)e^{-z(x_o)\tau} \qquad -2e^{-x^2}\tau\int_{\max(|x|,|x_o|)}^{x^+} e^{-z(y)\tau}dy$$

(4.76)

Results computed from equation (4.76) with a number of different initial conditions and barrier heights are illustrated in Figure 10 . The general content of the above equation is readily perceived; Hoare and Rahman (1976) have discussed it in detail, we may note that the Arrhenius law of reaction kinetics is expressed through the factor $\exp(-\exp(-x^{+2})\tau)$, x^{+2} representing a reduced activation energy and reaction proceeding in accordance with the equlibrium hypothesis.

Similarly the lower barrier problem can be

Figure 10



(a) (b) (c) (d)

Relaxation of various delta ensembles of Rayleigh test-particles in the presence of an absorbing barrier (equation (4.76).).

studied quite easily by the transform method.

Figure 10 shows the relaxation of various delta ensembles of Rayleigh test-particles in the presence of an absorbing barrier (equation (4.76)). Positions of initial delta function, x_o, and absorbing barrier, x^+, in the four cases are (a) x_o=0.0, x^+=1.5; (b) x_o= 0.5,x^+=1.0; (c) x_o=0.0, x^+=1.5; (d) x_o=1.0, x^+= 1.5.
The vertical arrows represent the decay of the delta function, its probability component scaled to unity by the dot. The column on the right represents the integrated flux over the barrier, scaled to unity by the horizontal bar. The figures give the elapsed time in reduced units. Note the interplay between three effective time-scales involving:

(i) the decay of the delta function
(ii) relaxation to the Gaussian
(iii) leakage across the barrier.

The distributions of the unabsorbed test-particles are effectively Gaussian for $\tau \approx 5.0$ in cases (a) to (c) and $\tau \approx 1.0$ in (d).

CHAPTER FIVE

SPATIAL TRANSPORT PROBLEM AND PHYSICAL PROPERTIES OF THE SPECIAL RAYLEIGH MODEL

Section 5.1. Introduction

In this chapter the investigation of the special Rayleigh model is continued through a treatment of the spatial transport problem. The coupled position-velocity distribution function of an inhomogeneous ensemble being, as in higher dimensional models, almost out of the question, we shall concentrate on the spatial moments, particularly as expressed through the Van Hove position-time correlation function $G(r,t)$. Our main explicit result will be the derivation of the second spatial moment $\langle r^2(t) \rangle$ and thus the expression for the coefficient of diffusion.

In case of condensed systems, it is usual to work in Gaussian approximation, first introduced by Vineyard (1958), in which $G(r,t)$ is assumed to be a Gaussian function of position at all times. This approximation is known to be exact at short times and long times for an arbitrary system (Rahman et al 1962), and at all times for an isotropic harmonic system. (Van Hove 1954.) Non-Gaussian behaviour has been considered by several authors(see e.g. Desai and Nelkin 1966). For monoatomic fluids, the corrections arise from dynamical considerations and have been studied in the classical limit, where $G(r,t)$ is the

probability per unit volume of finding an atom at position r and at time t, knowing that it was at origin at time t=o. In this chapter for the special model the non-Gaussian behaviour is examined in detail by considering the second and the fourth spatial moments. In the Gaussian approximation, the knowledge of the second spatial moment would be sufficient to determine all the higher spatial moments, however, the present calculations show that the non-Gaussian corrections at intermediate times are quite significant.

It is well known (see e.g. Kubo 1957) that the velocity autocorrelation function yields the self-diffusion coefficient for the test-particles. Thus it is very natural to consider in this chapter, the autocorrelation function and the second spatial moment which are closely related. To the approximations of the linear response theory, the admittance σ of an ensemble of Rayleigh test-particles, charge e , is related by a simple formula to the autocorrelation function. Hence, for the special model, together with the autocorrelation function, the electrical properties have been presented in this chapter.

In the next section all the interesting physical properties which can be obtained from the solution of the homogeneous equation (4.69) are calculated. The first velocity moment behaviour and the autocorrelation function can be obtained by considering only the odd component of the solution (4.69). Throughout we shall work with the fundamental initial condition $\delta(x-x_o)$ without loss of generality.In section four, the spatial problem is studied.

Section 5.2. Velocity-Moments and Autocorrelation Function

(a) Moment Relaxation

Consider first the relaxation of the first moment of the velocity distribution, $\langle x(\tau) \rangle$. Since

$$\langle x(\tau) \rangle = \int_{-\infty}^{\infty} dx\, xP(x,\tau) = 2 \int_{0}^{\infty} dx\, xP_{od}(x,\tau) \qquad (5.1)$$

we need perform an integration on the odd part of the solution. Taking first the particular case where $P(x,o) = \delta(x-x_o)$, we obtain by direct operation on the solution (4.69)

$$\langle x(\tau) | x_o \rangle = x_o \exp(-z(x_o)\tau) - 2(\mathrm{sgn}(x_o))\tau \int_{o}^{\infty} dx\, x\hat{h}_o(x) \int_{o}^{\min(|x|,|x_o|)} du\, e^{-z(u)\tau} + \hat{L}^{-1} \left\{ \frac{Q(x_o,s)}{Q(\infty,s)}\, 2 \int_{o}^{\infty} dx \hat{h}_o(x)\, Q(x,s) \right\}$$

$$(5.2)$$

By using the identity (see (3.13) and (3.14))

$$\frac{d}{dx}(xz'(x) - z(x)) = 2\, x\, \hat{h}_o(x) \qquad (5.3)$$

both the above integrals simplify on integration by parts:

$$2\mathrm{sgn}(x_o)\int_o^{\infty} dx\; x\,\hat{h}_o(x)\tau\int_o^{\min(|x|,|x_o|)} du\;\exp(-z(u)\tau)$$

$$= x_o e^{-z(x_o)\tau} - \int_o^{|x_o|} du(1 - \tau z(u))\exp(-z(u)\tau)$$

(5.4)

and

$$2\int_o^{\infty} dx\; x\hat{h}_o(x)\; Q(x,s) = \left[\frac{1}{\pi^{\frac{1}{2}}} - sQ(\infty,s)\right]$$

(5.5)

with the result that

$$\langle x(\tau)|\, x_o\rangle = \int_o^{x_o} du(1 - z(u)\tau)\exp(-z(u)\tau)$$

$$+ \hat{L}^{-1}\left\{\frac{Q(x_o,s)}{Q(\infty,s)}\left(1/\pi^{\frac{1}{2}} - sQ(\infty,s)\right)\right\}$$

(5.6)

However, since by the derivative theorem for Laplace transforms

$$sQ(x,s) = \hat{L}\left\{\frac{\partial}{\partial\tau}\cdot\tau\int_o^{x_o} dy\;\exp(-z(y)\tau)\right\} \qquad (5.7)$$

the first integral cancels with the second term in the inverse and we obtain the simple result

$$\langle x(\tau)|\, x_o\rangle = (1/\pi^{\frac{1}{2}})\;\hat{L}^{-1}\left\{\frac{Q(x_o,s)}{Q(\infty,s)}\right\} \qquad (5.8)$$

We may note that the identity (5.5) above leads to

$$\underset{s \longrightarrow \infty}{\text{Limit}} \quad sQ(\infty, s) = \frac{1}{\pi^{\frac{1}{2}}} \qquad (5.9)$$

which guarantees the correct initial-value result $\langle x(o) | x_o \rangle = x_o$ and the multiplication of $Q(x_o, s)/Q(\infty, s)$ by s and taking the limit as s tends to zero confirms that $\langle x(\infty) | x_o \rangle = o$ for all x_o. Similar result for an arbitrary initial condition may be obtained by superposition.

By applying the method of finding the inverse transforms involving the function $Q(x,s)$, developed in chapter four (see Appendix D), we can write

$$\langle x(\tau) | x_o \rangle = \frac{1}{\pi^{\frac{1}{2}}} \int_o^\infty dx_\lambda z'(x_\lambda) \frac{\exp(-z(x_\lambda)\tau)}{A(\lambda)} \Big(R(x_o,\lambda) g(\infty,\lambda) - R(\infty,\lambda) g(x_o,\lambda) \Big) \qquad (5.10)$$

The above result can be obtained by using equation (4.66) which expresses $P_{od}(x,\tau)$ in terms of eigendistribution:

$$xP_{od}(x,\tau) = \int_o^\infty dx_\lambda z'(x_\lambda) e^{-z(x_\lambda)\tau} \frac{g(\infty,\lambda)}{A(\lambda)} \left(R(x_o,\lambda) - \frac{g(x_o,\lambda) R(\infty,\lambda)}{g(\infty,\lambda)} \right) \cdot x \hat{h}_o(x) \left(R(x,\lambda) - \frac{g(x,\lambda) R(\infty,\lambda)}{g(\infty,\lambda)} \right) \qquad (5.11)$$

By using the identity (5.3) we can show that

$$2\int_0^\infty dx\, \hat{h}_o(x)x\left(R(x,\lambda)-\frac{g(x,\lambda)R(\infty,\lambda)}{g(\infty,\lambda)}\right) = \frac{1}{\pi^{\frac{1}{2}}} \qquad (5.12)$$

Therefore,

$$\langle x(\tau)|x_o\rangle = \frac{1}{\pi^{\frac{1}{2}}}\int_0^\infty dx_\lambda z'(x_\lambda)e^{-z(x_\lambda)\tau}\frac{g(\infty,\lambda)}{A(\lambda)}\left[R(x_o,\lambda) - \frac{g(x_o,\lambda)R(\infty,\lambda)}{g(\infty,\lambda)}\right] \qquad (5.13)$$

which is identical to equation (5.10). From computational point of view, it is more convenient to use (5.8) rather than the above expression for the first velocity moment.

(b) The Velocity Autocorrelation Function

A similar simplification occurs on writing the velocity autocorrelation function $S_x(\tau)$. Defining

$$S_x(\tau) = 2\int_0^\infty x_o\hat{h}_o(x_o)\langle x(\tau)|x_o\rangle dx_o \qquad (5.14)$$

we have

$$S_x(\tau) = \frac{2}{\pi}\hat{L}^{-1}\left\{\frac{1}{Q(\infty,s)}\int_0^\infty x_o\hat{h}_o(x_o)Q(x_o,s)\,dx_o\right\} \qquad (5.15)$$

Using (5.5) once again, we have

$$S_x(\tau) = (1/\pi)\,\hat{L}^{-1}\,(1/Q(\infty,s)\pi^{\frac{1}{2}} - s) \qquad (5.16)$$

the same analysis as before showing that the inverse is, in spite of its appearance, non-singular This equation leads to an efficient computation of $S_x(\tau)$, the results of which we present in the next section.

By using the expression (5.13) for the first velocity moment, we can write

$$S_x(\tau) = (1/\pi)\int_0^\infty dx_\lambda z'(x_\lambda)e^{-z(x_\lambda)\tau}g(\infty,\lambda)/A(\lambda)$$

$$2\int_0^\infty dx_o \hat{h}_o(x_o)x_o\Big(R(x,\lambda) - \frac{g(x_o,\lambda)R(\infty,\lambda)}{g(\infty,\lambda)} \Big)$$

(5.17)

Using (5.12) once again, we have

$$S_x(\tau) = (1/\pi^{\frac{1}{2}})^3 \int_0^\infty dx_\lambda\; z'(x_\lambda)\; g(\infty,\lambda)/(R(\infty,\lambda)^2 + \pi^2 g(\infty,\lambda)^2) \cdot \exp(-z(x_\lambda)\tau)$$

(5.18)

the same expression is obtained if one finds the inverse transform in equation (5.16) in the usual way.

In the next sub-section, asymptotic analysis for $S_x(\tau)$ is presented.

(c) Asymptotic Analysis

To obtain the autocorrelation behaviour at long times, we must expose the limiting form of (5.16) as $s \longrightarrow o$. It is simplest if we work in the time variable and note that asymptotically:

$$\int_o^\infty du \exp(-z(u)\tau) \underset{\tau \to \infty}{\sim} \frac{1}{2} (\pi/\hat{h}_o(o))^{\frac{1}{2}} \tau^{-\frac{1}{2}} e^{-\tau}$$

by virtue of the relationship

$$z(x) = 1 + \hat{h}_o(o)x^2 + O(x^4)$$

Furthermore,

$$\frac{d}{d\tau}\left[\tau \int_o^\infty e^{-z(u)\tau} du\right] \underset{\tau \to \infty}{\sim} \frac{1}{2}\left[(\pi/\hat{h}_o(o))^{\frac{1}{2}} e^{-\tau}(1-2\tau)\tau^{-\frac{1}{2}}\right]$$

Now the Laplace transform of the right-hand side exists and is equal to $(\pi/4(\hat{h}_o(o))^{\frac{1}{2}}) s(s+1)^{-3/2}$ From this we can deduce that the $s \longrightarrow o$ behaviour of $Q(\infty, s)$ is

$$Q(\infty, s) \underset{s \to o}{\sim} \pi/4(\hat{h}_o(o))^{\frac{1}{2}} . (s+1)^{-3/2} \qquad (5.19)$$

Since the reciprocal of this dominates the term s on the right-hand side of (5.16) we may assert that the Laplace transform of $S_x(\tau)$ is formally

$$S_x(\tau) \underset{\tau \to \infty}{\sim} 4\hat{h}_o(o)^{\frac{1}{2}} \pi^{-5/2} . \hat{L}^{-1}(s+1)^{3/2} \qquad (5.20)$$

While the inverse of the right-hand side does not exist in the ordinary sense, it does in the realm of distributions, where we have the following

$$L\,(\mathrm{Pf}.\,\tau^{-5/2} e^{-\tau}) = \frac{4\pi^{\frac{1}{2}}}{3}(s+1)^{3/2} \qquad (5.21)$$

Here Pf. denotes the pseudofunction corresponding to the Hadamard finite part of the Laplace integral (see e.g. Zemanian (1965) especially chap.8 and item 31, table B.2). This interpretation is both adequate and natural in the present problem where we simply wish to supress the influence of an irrelevant singularity at zero time. Thus we can state unequivocally that

$$S_x(\tau) \underset{\tau\to\infty}{\sim} \frac{3}{\pi^3}(\hat{h}_0(o))^{\frac{1}{2}} \tau^{-5/2}\ e^{-\tau} \qquad (5.22)$$

From this it is clear that the nature of the heat-bath affects asymptotic behaviour only through a constant factor, the $\tau^{-5/2}\ e^{-\tau}$ being, it would seem, a universal feature of the special Rayleigh model. The factor $e^{-\tau}$ in (5.22) exhibits the Markovian behaviour of the model and prevents the existence of the so called ' long-time tail '.

(d) Self-diffusion

By a well-known formula (Kubo 1957) the velocity autocorrelation function yields the self-diffusion coefficient D for

test-particles. Thus

$$D_o = \int_o^\infty S_x(\tau)d\tau = \underset{s \longrightarrow o}{\text{Limit}}\ L\ (\ S_x(s)\ ) \qquad (\ 5.23\ )$$

From this it follows that, for a Rayleigh test-particle,

$$D_o = \pi^{-3/2}\ \underset{s \longrightarrow o}{\text{Limit}}\ (\ Q(\omega,s)\ )^{-1} = \pi^{-3/2}\cdot\left[\int_o^\infty \frac{dy}{z(y)^2}\right]^{-1} \qquad (\ 5.24\ )$$

A numerical evaluation of the integral for the Maxwellian heat-bath ($z(x)=\exp(-x^2) + \pi^{\frac{1}{2}}x\,\mathrm{erf}(x)$) gave the value $D_o = 0.185164.....$ in dimensionless τ time-scale. Reverting to the unscaled units, this is found to be equivalent to the formula

$$D = 1.827495.....(na)^{-1}(2k_BT/\pi m)^{\frac{1}{2}} \qquad (\ 5.25\ )$$

Here the algebraic factor is simply the mean-free-path approximation to D in one dimension, n being the number-density of test-particles and a their effective cross-section. The increase over the MFP value would seem to reflect a more just account of the contribution from particles in the high-velocity tail of the Maxwellian.

(e) Electrical Conductivity

To the approximations of linear response theory we may express the admittance, σ, of an ensemble of Rayleigh test-particles,

charge e, by the formula

$$(\sigma/\sigma_o) = (1/D_o) \int_o^\infty \exp(i\omega\tau) S_x(\tau) \qquad (5.26)$$

Here $S_x(\tau)$ is the dimensionless velocity autocorrelation function as throughout, D_o the corresponding diffusion coefficient (5.24), and σ_o is the conductivity ($\omega \longrightarrow o$). Scaling is then through the Stokes-Einstein relationship $\sigma_o = (De^2/k_BT)$ with D given by (5.25). Thus we need only to substitute $-i\omega$ for s in the Laplace transform expression (5.16) to obtain

$$\sigma(\omega) = (\sigma_o/D_o\pi). \left(\pi^{-\frac{1}{2}} Q(\infty,-i\omega)^{-1} + i\omega \right) \qquad (5.27)$$

From this the real and imaginary parts of σ may be obtained explicitly. Noting that

$$Q(\infty,-i\omega)^2 = \left[\int_o^\infty \frac{z(u)^2-\omega^2}{(z(u)^2+\omega^2)^2} du \right]^2 + 4\omega^2 \left[\int_o^\infty \frac{z(u)du}{(z(u)^2+\omega^2)^2} \right]^2 \qquad (5.28)$$

it follows that

$$Re(\sigma) = \rho_o/|Q(\infty,-i\omega)|^2 \cdot \int_o^\infty \frac{z(u)^2-\omega^2}{(z(u)^2+\omega^2)^2} du \qquad (5.29)$$

and

$$\mathrm{Im}(\sigma) = \pi^{\frac{1}{2}}\rho_o\omega/|Q(\infty,-i\omega)|^2\left(1 - 2.\int_o^\infty \frac{du\ z(u)}{(z(u)^2+\omega^2)^2}\right) \qquad (5.30)$$

where by definition

$$\rho_o = (\sigma_o/D_o\pi^{3/2}) \qquad (5.31)$$

Thus we observe the expected decay of the conductance $\mathrm{Re}(\sigma)$ from the Stokes-Einstein value under dc conditions to zero at high frequencies. The frequency-response shows a broad decay with no tendency to resonance. The phase-lag can be seen to tend to 90^o at high frequencies ($\arctan\left[\mathrm{Im}(\sigma)/\mathrm{Re}(\sigma)\right] \longrightarrow \frac{\pi}{2}$ as $\omega \longrightarrow \infty$). Numerical computations of the above quantities are discussed in the next section.

(f) Autocorrelation of Speed

The speed autocorrelation function $S_{|x|}(\tau)$ is of lesser interest that the velocity autocorrelation function, but can be found explicitly by integrations over the even part of the velocity distribution, (4.69). We find after some partial integrations

$$\langle |x|(\tau)|\, x_o\rangle = \pi^{-\frac{1}{2}} \int_{|x_o|}^\infty \left[(z(y)-1)\tau - 1\right]\cdot\exp(-z(y)\tau)\, dy \qquad (5.32)$$

and

$$S_{|x|}(\tau) = \pi^{-\frac{1}{2}} \int_0^\infty e^{-z(y)\tau} \left[(z(y) - 1)\tau - 1) \cdot \left(1 - \hat{h}_o(y) - \pi^{-\frac{1}{2}} z'(y)\right) \right] dy \qquad (5.33)$$

$\langle |x|(\tau) | x_o \rangle$ being the relaxation of mean speed from an initial delta-distribution at x_o. The essentially non-exponential character of both functions is quite clear.

Section 5. 3. Numerical Computations

The numerical inversion of Laplace transforms is nowadays a straightforward procedure and a number of excellent algorithms are available. We were thus able to calculate the inverse function $\hat{L}^{-1}\{\ \}$ in (5.16) and (4.69) to an accuracy quite sufficient for illustration of the behaviour of the solutions under various conditions. The method we employed was the Dubner-Abate procedure as improved by Durbin and Crump (Dubner and Abate 1968; Durbin 1974; Crump 1976). Although the algorithms referred to are now reasonably well-known in the computing literature, it is unlikely that they have often been used with functions as complicated as those which arise here. We found it necessary to speed the convergence of the integrals by use of bounding approximations and the so called ' ε-algorithms' to improve the convergence of the Fourier series involved (see Shanks(1955), Wynn (1956)).

It will suffice here to present a small selection of results designed to illustrate the main characterics of the

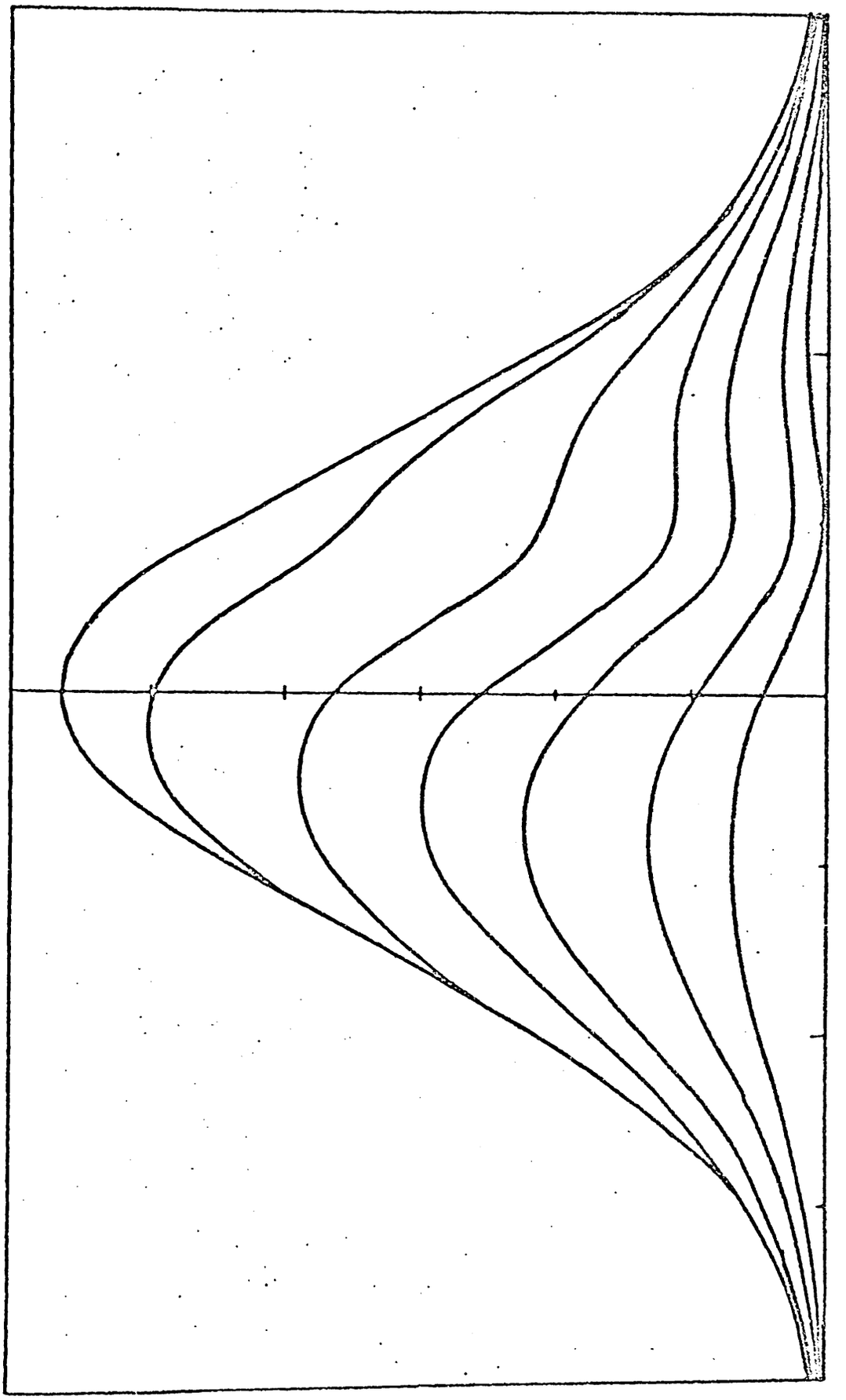


Figure 11a: P(x,τ) with the initial condition P(x,o) = δ(x-0.5)

τ=0.1 ; 0.2 ; 0.4 ; 0.6 ; 1.0 ; 2.0 ; ∞.

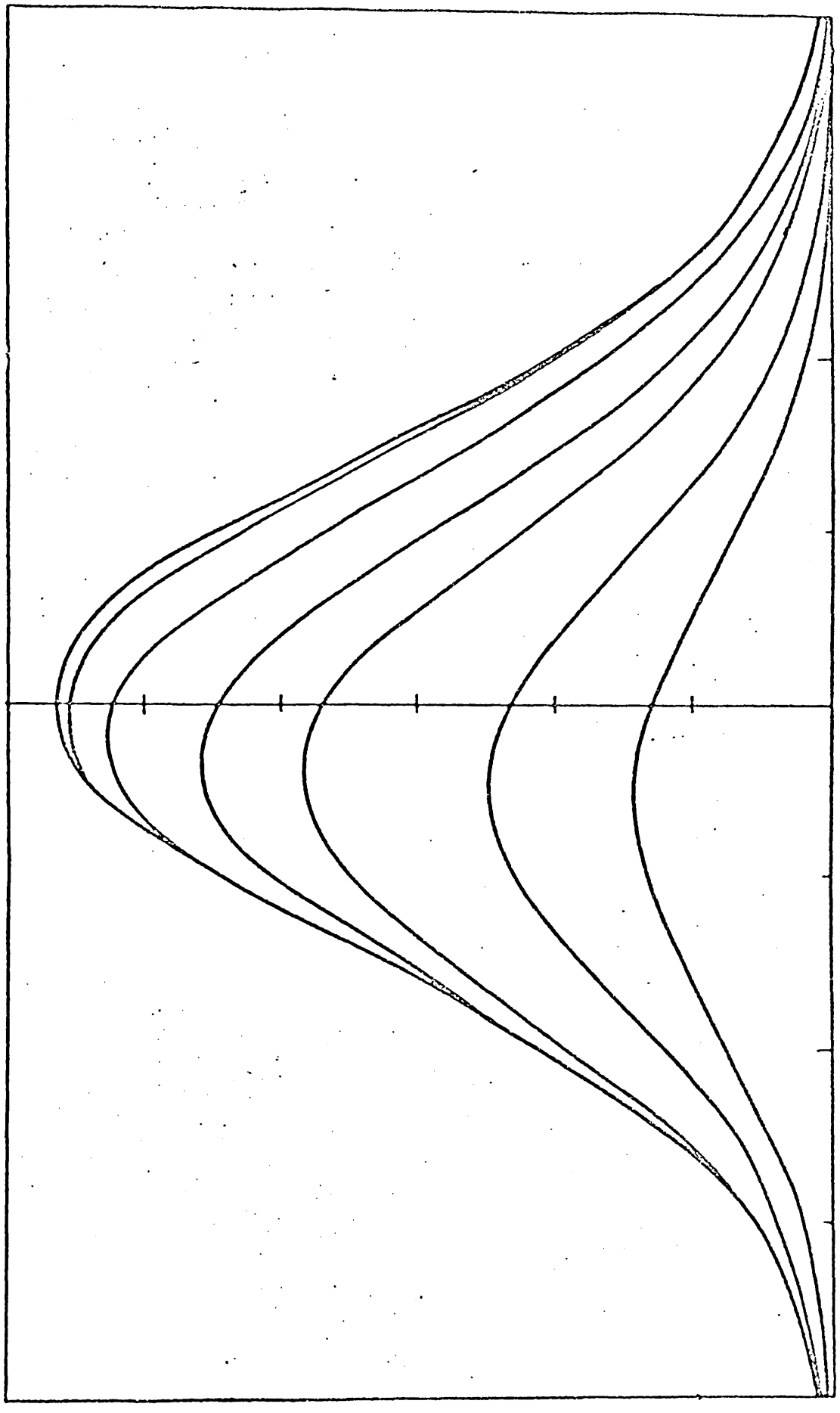


Figure 11b: P(x,τ) with the initial condition P(x,o) = δ(x-1.5)

initial-value and autocorrelation solutions and the electrical conductivity.

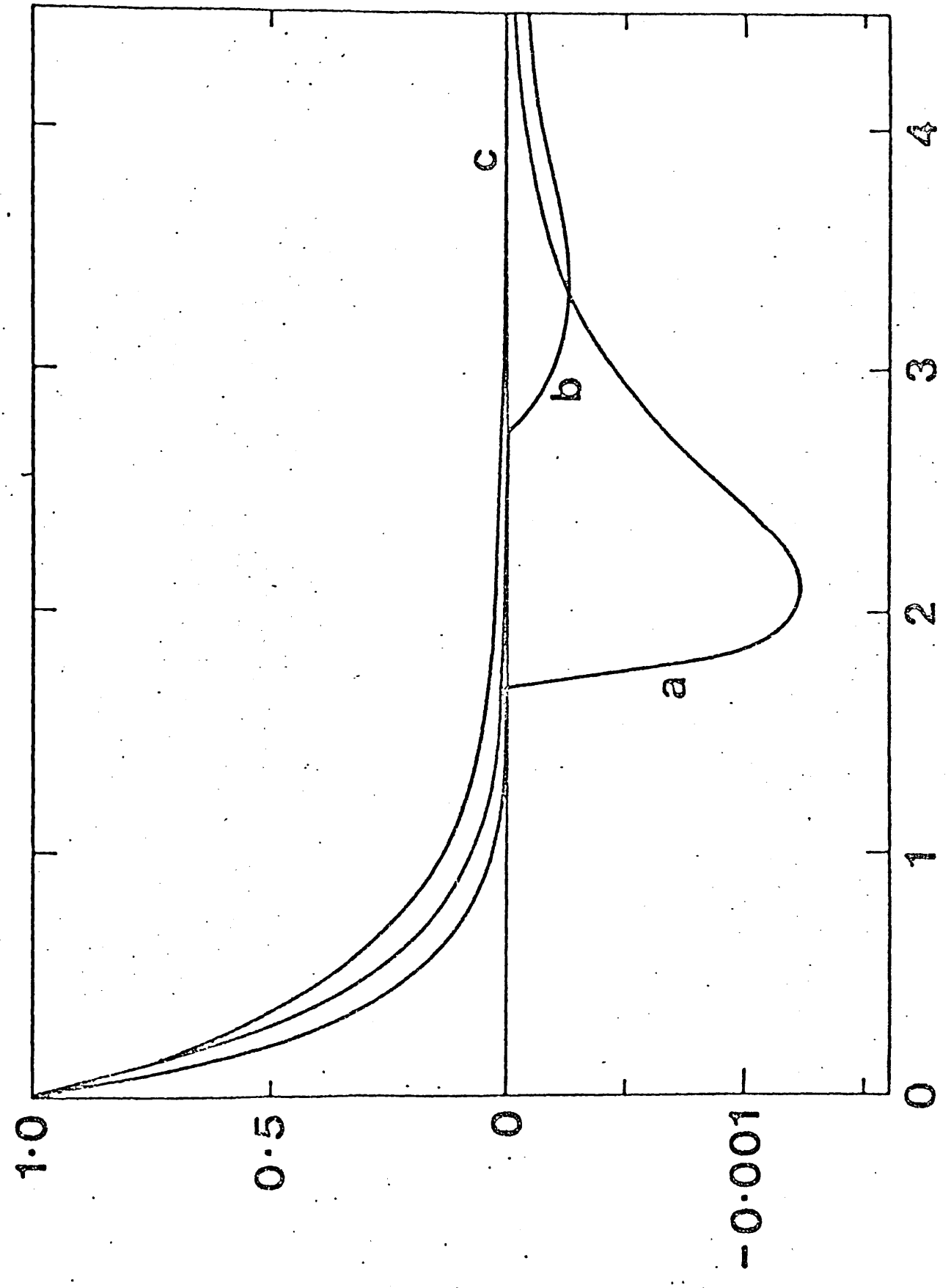
(a) Initial-value Solutions

Figure 11 shows full-range initial value solutions under delta-function conditions $P(x,o)=\delta(x-x_o)$ with $x_o = 0.5$ and 1.5 respectively. Anumber of features are quite marked, notably the asymmetry of the regular part of the distribution at all finite times, with a drift of the most probable velocity from approximately x_o to zero as the relaxation progresses. The physical origin of this is clear: there is an anticorrelation in velocity after the first collision of each test-particle, due, it would seem, to the enhanced probability of a'head-on' collision for particles in the initial delta-function. A related feature is the emergence of a pronounced ' shoulder ' in the vicinity of x_o when x_o is relatively large—— presumably due to an appreciable contribution from test particles which have collided twice within the order of a single collision-time. Note that the parity components P_{od} and P_{ev} are easily estimated by the visual trick of reflecting the left-hand half onto the right and summing or differencing as appropriate. In this way the main feature of the speed-relaxation $P(|x|,\tau)$ can be distinguished—a distinct lag in the equilibrium of test-particles with near-zero velocities relative to those in the high-energy 'tail' of the distribution.

(b) Mean Velocities

The mean velocity relaxation according to (5.8) is

Figure 12: Relaxation of mean velocity for different initial delta-distributions. $P(x,o)=\delta(x-x_o)$. Curves:(a) $x_o=1.5$,(b) $x_o=1.0$,(c) $x_o=0.5$.The lower half shows the small negative flux which develpos in a direction opposite to the initial delta-function.



interesting in that, depending on the initial conditions, the average $\langle x(\tau) \rangle$ may possibly become negative, indicating that a net flux develops in the direction contrary to that of the initial distribution. Figure 12 shows that such a reversed flux can occur to a slight degree under certain conditions.

(c) Autocorrelation

Our most interesting result is perhaps the computation of the full velocity autocorrelation function $S_x(\tau)$ for equilibrium fluctuations according to (5.16) . The function, $S_x(\tau)$ computed by numerical inversion is shown by Figure 13 . It is clear that the decay of fluctuations is very nearly exponential in appearance, though the mathematical behaviour cannot at any time be strictly described in this way. The asymptotic form of $S_x(\tau)$ predicted by (5.22) (dashed curve) gives a fairly good estimate of the true one, though with a very slow numerical convergence. Thus the numerical results both confirm and deny the contention of Cukier and Hynes (1976) that all model processes yield effectively exponential decay. Numerically, it is true that the exact function can be approximated, moderately well by a single exponential decay constant; nevertheless this behaviour can be given no analytic significance in any time-regime. In particular, the approximation advanced by Cukier and Hynes—— that of taking the initial slope $(\partial S_x(\tau)/\partial \tau)_{\tau=0}$ to determine the general exponential behaviour—— is clearly a poor one in terms of the results of Figure 13 . The absence of exponential decay, even at long times, is

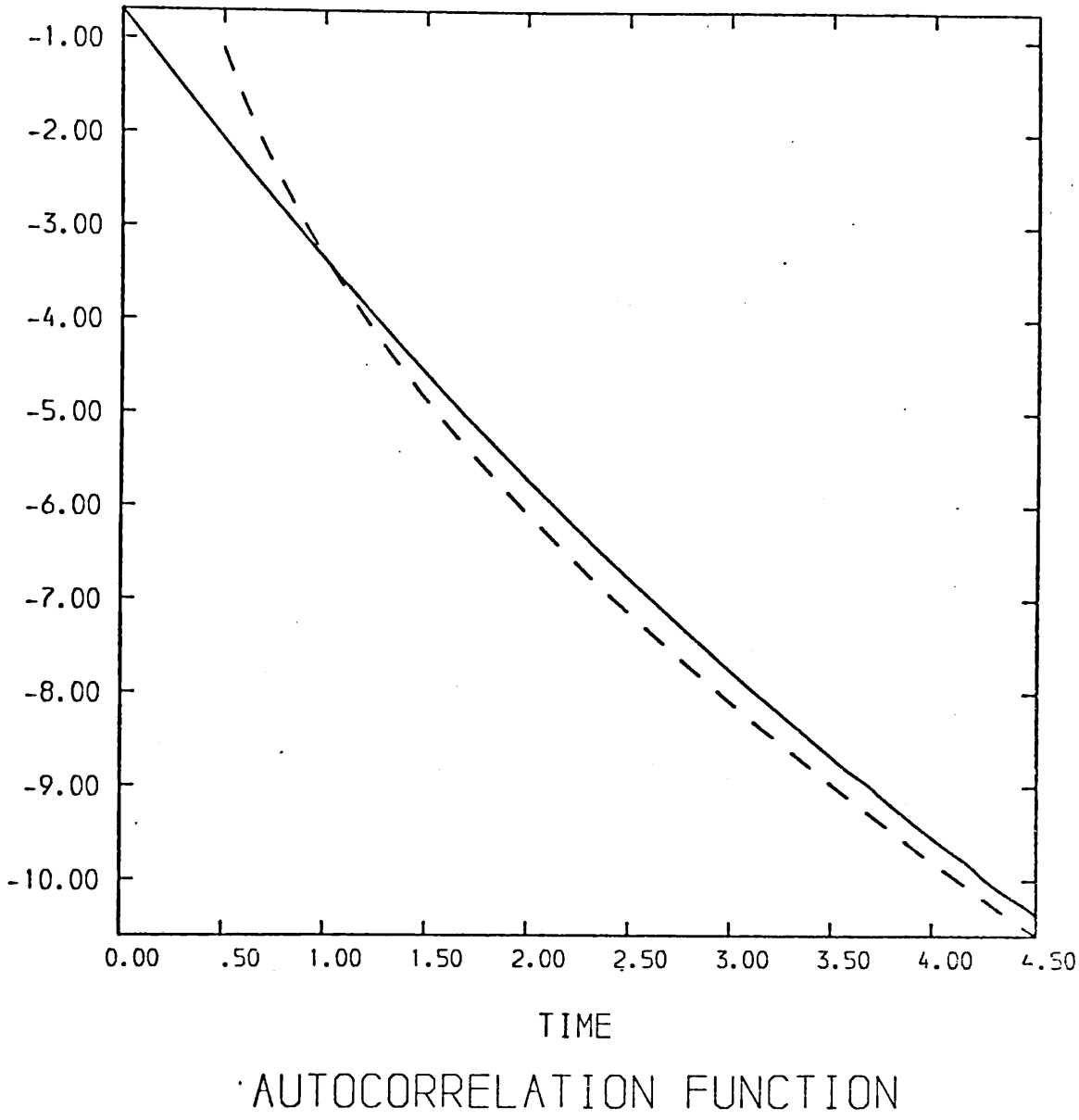


Figure 13 The Velocity autocorrelation function for equlibrium fluctuations in an ensemble of Rayleigh test-particles.The solid line is the the result obtained by numerical inversion of expression in (5.16). The dashed line shows the asymptotic approximation (5.22). (All the results are calculated for the Maxwellian heat-bath.)

noteworthy but hardly surprising in a system known to posses an unbounded continuum spectrum for the underlying transition operator.

(d) Electrical Conductivity

The real and imaginary parts of the complex admittance σ may be computed directly from equation (5.27) as a function of the frequency of the applied field.(We do not, of course, program the expressions (5.29) and (5.30) directly, it suffices to use a complex FORTRAN version of the numerical quadrature for the $Q(x,s)$ integrals already available, working with equation (5.27) throughout) The results, plotted in dimensionless form in Figure 14 are seen to correspond broadly to physical intuition. Thus the dissipative component $\{ Re(\sigma) \}$ representing the transmission of energy to the heat-bath, is maximum under D.C. conditions and falls with a bell-shaped decay to zero at high-frequencies. There is no sign of resonance and frequencies very high compared to the mean collision frequency are required for the dissipation to be effectively zero. As deduced earlier, the current lags behind the applied field, its phase angle increasing regularly from zero to 90^{o} at infinite frequency.

Figure 14a: Real and Imaginary parts of the admittance function for charged Rayleigh test-particles (solid and broken lines respectively). Results are for a Maxwellian heat-bath. The o-scale in arbitrary units applies to both the curves. The real component is proportional to energy dissipation into the heat-bath per cycle.

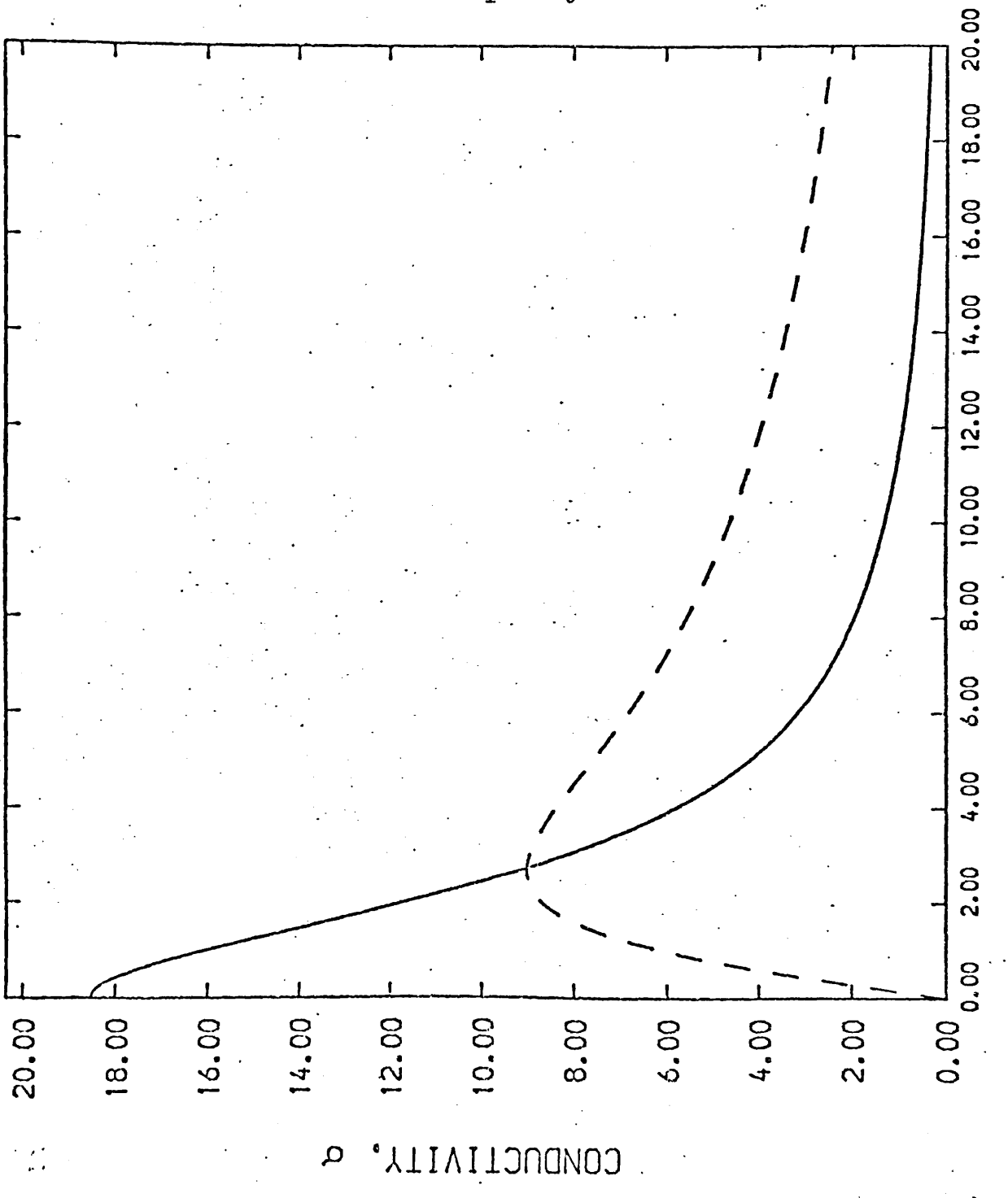


Figure 14b: Current in a charged Rayleigh System as a function of frequency.(Maxwellian Heat-bath.)

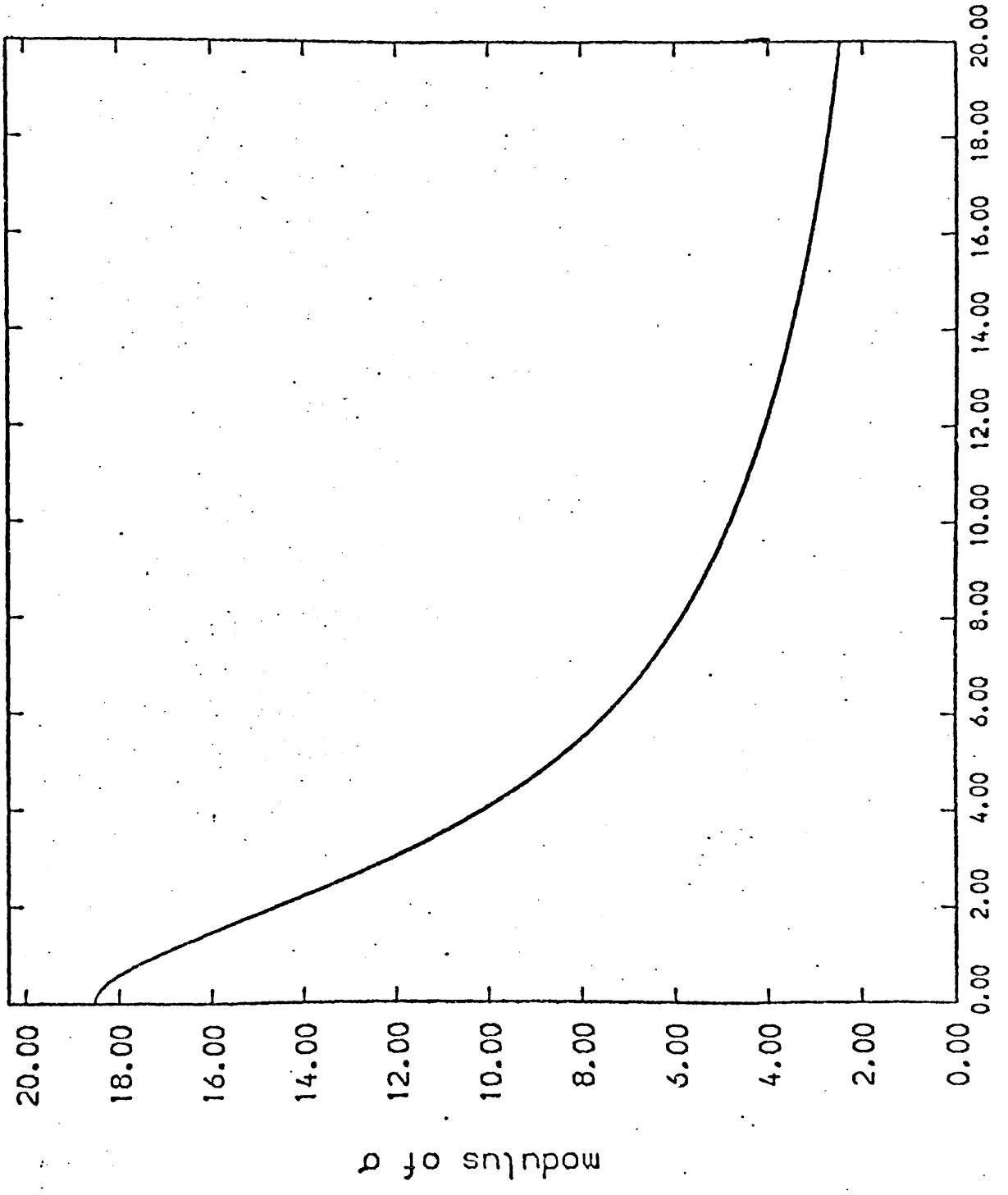
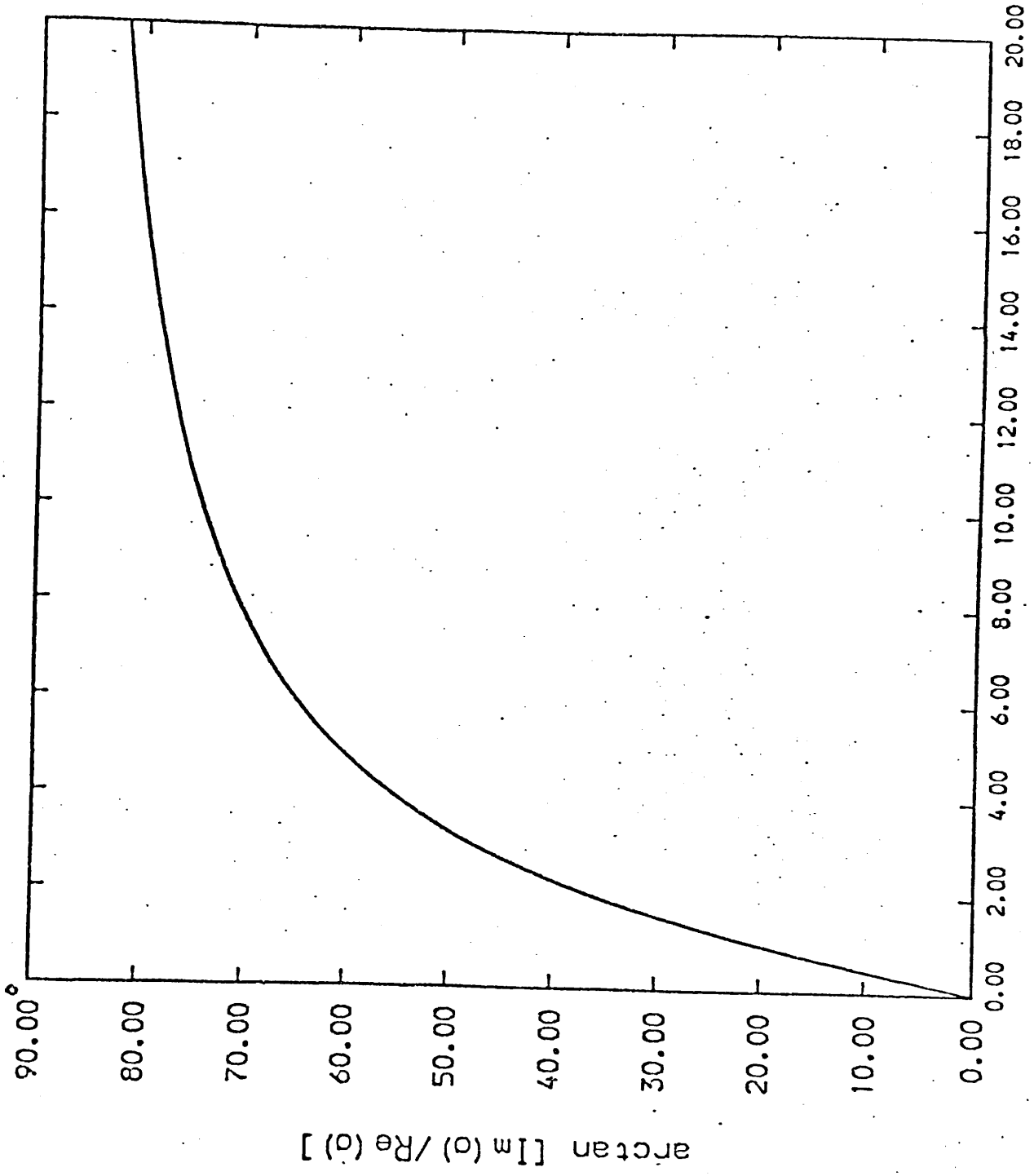


Figure 14c Response lag in a charged Rayleigh system as a function of frequency (Maxwellian heat-bath).



Section 5.4. Spatial Transport Problem

The linear and one dimensional character of the special Rayleigh model leads to a relatively simple equation for the spatial evolution of a test-particle ensemble. Designating by $P(r,V,t)$ the velocity-position distribution function for particles at time t, the conservation of probability can be expressed by the integrodifferential equation

$$\frac{\partial}{\partial t}P(r,V,t) + V.\frac{\partial}{\partial r}P(r,V,t) = \int_{-\infty}^{\infty} dV'K(V'|V)P(r,V',t) - Z(V)P(r,V,t) \qquad (5.34)$$

where, as in the case of the homogeneous problem,

$$K(V|V') = C|V-V'|h_o(V') \qquad (5.35)$$

and

$$Z(V) = \int_{-\infty}^{\infty} dV'K(V|V') \qquad (5.36)$$

The above equation is a Markovian Equation with a streaming term added on the left-hand side. As before $K(V|V')$ is the scattering kernel in velocities and $Z(V)$ the velocity-dependent collision number, its integral over all final states. Sources and absorbers are assumed to be absent and infinite medium boundary conditions are imposed. An initial distribution $P(r,V,o)$ is assumed given and this may be normalised either absolutely or, if it is periodic, over a characteristic

distance. Since we shall only be interested in an initially localised ensemble, we choose the former alternative and write

$$\iint dr\,dV\; P(r,V,t) \;=\; 1 \qquad (5.37)$$

As usual we make an immediate transformation to reduced variables:

$$\begin{aligned} x &= (C/\pi^{\frac{1}{2}}).\, r \\ v &= (1/\pi^{\frac{1}{2}}\bar{V}_o).\, V \\ \tau &= C\,\bar{V}_o.\, t \;=\; Z(0).t \end{aligned} \qquad (5.38)$$

with the consequence that

$$P(x,v,\tau) \;=\; (\pi\bar{V}_o/C).\, P\left((C/\pi^{\frac{1}{2}})^{-1}.x,\; (\pi^{\frac{1}{2}}\bar{V}_o).v,\; \tau/Z(0)\right) \qquad (5.39)$$

and

$$\iint dx\,dv\; P(x,v,\tau) \;=\; 1 \qquad (5.39)$$

In terms of the reduced variables, the transport equation assumes the form:

$$\frac{\partial}{\partial\tau}P(x,v,\tau) + v.\frac{\partial}{\partial x}P(x,v,\tau) + z(v)P(x,v,\tau) = \hat{h}_o(v)\int_{-\infty}^{\infty} dv'\,|v-v'|\;P(x,v',\tau) \qquad (5.40)$$

where

$$z(v) = \int_{-\infty}^{\infty} dv' \, |v-v'| \, h_o(v') \qquad (5.41)$$

and

$$\hat{h}_o(v) = \pi \bar{V}_o \cdot h_o(\pi^{\frac{1}{2}} \bar{V}_o \cdot v) \qquad (5.42)$$

(see (3.8).)

Since the Van Hove function $G(r,t)$ is the probability per unit length (or volume in three dimensions) for finding a test-particle at position r at time t if the same test-particle is known to have been at the origin at time zero, and since we must sample an ensemble of systems at thermal equlibrium tc determine $G(r,t)$, the appropriate initial condition is

$$P(x,v,o) = \delta(x) . \hat{h}_o(v)/\pi^{\frac{1}{2}} \qquad (5.43)$$

We can work with the fundamental initial condition $\delta(x-x_o)\delta(v-v_o)$ and then use the principle of superposition but as we shall see below it is much simpler to work with the above initial condition from the begining.

In reduced variables the Van Hove function can be written in the form

$$G(x,\tau) = \pi^{\frac{1}{2}}/C \, . \, G(r,t) \qquad (5.44)$$

where

$$G(x,\tau) = \int_{-\infty}^{\infty} dv \, P(x,v,\tau) \qquad (5.45)$$

From equation (5.43) and (5.45) we see that $G(x,\tau)$ has the required general properties

$$G(x,o) = \delta(x) \qquad (5.46)$$

and

$$\int_{-\infty}^{\infty} dx G(x,\tau) = 1. \qquad (5.47)$$

By introducing the spatial Fourier transform of the position-velocity density

$$h(k,v,\tau) = 1/2\pi \int_{-\infty}^{\infty} dx e^{-ikx} P(x,v,\tau) \qquad (5.48)$$

the spatial transport equation becomes

$$\left(\frac{\partial}{\partial \tau} + ikv + z(v) \right).h(k,v,\tau) = \hat{h}_o(v) \int_{-\infty}^{\infty} dv' |v-v'| h(k,v',\tau) \qquad (5.49)$$

with the initial condition

$$h(k,v,o) = \hat{h}_o(v)/2\pi^{3/2} \qquad (5.50)$$

In order to proceed further it is convenient to adopt the terminology used in the neutron transport theory (see e.g. Nelkin and Ghatak 1964). In most problems in neutron scattering it is more convenient to deal with the so-called intermediate scattering function

$$\mathcal{H}(k,\tau) = \int_{-\infty}^{\infty} h(k,v,\tau) dv \qquad (5.51)$$

with the general property

$$\mathcal{H}(k,o) = \mathcal{H}(o,\tau) = 1/2\pi \qquad (5.52)$$

A quantity of direct physical interest in neutron scattering experiment is the differential energy transfer cross section

$$S(k,\omega) = \int_0^\infty d\tau \exp(-i\omega\tau)\, \mathcal{H}(k,\tau) \qquad (5.53)$$

which is the double Fourier transform of the Van Hove function $G(x,\tau)$. Since $\mathcal{H}(k,\tau)$ is determined from an initial value problem, we must specify its behaviour for negative times in order to completely define $S(k,\omega)$. For a classical system, $S(k,\omega)$ is an even function of ω and $\mathcal{H}(k,\tau)$ is a real even function of time. Introducing the Laplace transform of $h(k,v,\tau)$ in the form

$$h(k,v,s) = \int_0^\infty d\tau \exp(-s\tau) h(k,v,\tau) \qquad (5.54)$$

and the transform of $\mathcal{H}(k,\tau)$ in the form

$$Q(k,s) = \int_0^\infty d\tau \exp(-s\tau)\, \mathcal{H}(k,\tau) \qquad (5.55)$$

we have

$$S(k,\omega) = Q(k,-i\omega) + Q(k,i\omega) \qquad (5.56)$$

where

$$Q(k,s) = \int_{-\infty}^\infty dv\, h(k,v,s) \qquad (5.57)$$

and $h(k,v,s)$ is the solution of the equation

$$(z(v) + ikv + s).h(k,v,s) = \hat{h}_o(v) \int_{-\infty}^{\infty} dv' |v-v'| h(k,v',s) + \hat{h}_o(v)/2\pi^{3/2} \qquad (5.58)$$

Having completed the formal preliminaries, we now turn to actual calculations.

In order to make the calculations simpler, it is convenient to define:

$$f(k,v,s) = h(k,v,s)/\hat{h}_o(v) \qquad (5.59)$$

in terms of which we can rewrite (5.58) in the simple form:

$$(z(v) + ikv + s).f(k,v,s) = \int_{-\infty}^{\infty} dv' |v-v'| \hat{h}_o(v') f(k,v,s) + 1/2\pi^{3/2} \qquad (5.60)$$

Partial differentiating (5.60) once with respect to v, we have

$$(z'(v)+ik)f(k,v,s) + (z(v)+ikv+s)f'(k,v,s) = \int_{-\infty}^{\infty} dv' sgn(v-v') \hat{h}_o(v') f(k,v',s) \qquad (5.61)$$

Partial differentiating (5.61) once with respect to v, we have

$$2(z'(v)+ik).f'(k,v,s) + (z(v)+ikv+s).f''(k,v,s) = o. \qquad (5.62)$$

The above equation can be integrated to give

$$f(k,v,s) = A(s,k) + B(s,k). \int_o^v du/(z(u)+iku+s)^2 \qquad (5.63)$$

To find the functions of integration A(s,k) and B(s,k), one has to substitute f(k,v,s) into (5.60) and (5.61) respectively and put v=o in the resulting expressions. In order to carry out this procedure, the following identities are required:

$$\frac{\partial}{\partial v}\left[(z'(v)+ik). \int_o^v du/(z(u)+iku+s)^2 + 1/(z(v)+ikv+s) \right] = z''(v). \int_o^v du/(z(u)+iku+s)^2 \qquad (5.64)$$

$$\frac{\partial}{\partial v}\left[v/(z(v)+ikv+s) - (z(v)-vz'(v)+s). \int_o^v du/(z(u)+iku+s)^2 \right] = vz''(v). \int_o^v du/(z(u)+iku+s)^2 \qquad (5.65)$$

By using the above identities we have:

$$I_a = \int_{-\infty}^{\infty} dv\,|v|\hat{h}_o(v). \int_o^v du/(z(u)+iku+s)^2$$

$$= \int_o^{\infty} dv v\hat{h}_o(v). \int_o^v du/(z(u)+iku+s)^2$$

$$- \int_o^{\infty} dv v\hat{h}_o(v). \int_o^v du/(z(u)-iku+s)^2$$

(using (5.65).)

$$= -\alpha_1 \qquad (5.66)$$

where

$$\alpha_1 = ik/(\pi+k^2) + \frac{s}{2}\left[\int_o^{\infty} du/(z(u)+iku+s)^2 - \int_o^{\infty} du/(z(u)+iku+s)^2\right] \qquad (5.67)$$

From equation (5.60) we obtain by setting v=o

$$(1+s)A(s,k) = B(s,k).I_a + A(s,k) + 1/2\pi^{3/2}$$

or

$$sA(s,k) = -\alpha_1 . B(s,k) + 1/2\pi^{3/2} \qquad (5.68)$$

where we have used the properties of the collision function z(x) (see (5.3)).

From equation (5.61) we obtain

by setting v=o

$$ikA(s,k) + B(s,k)/(1+s) = -\int_{-\infty}^{\infty} dv' sgn(v')\hat{h}_o(v')f(k,v',s)$$

$$= -I_b \qquad (5.69)$$

$$I_b = \int_{-\infty}^{\infty} dv' sgn(v')\hat{h}_o(v')f(k,v',s)$$

$$= B(s,k).\ \alpha_2 \qquad (5.70)$$

where

$$\alpha_2 = \int_{-\infty}^{\infty} dv' sgn(v')\hat{h}_o(v').\ \int_o^{v'} du/(z(u)+iku+s)^2$$

$$= \int_o^{\infty} dv'\hat{h}_o(v').\ \int_o^{v'} du/(z(u)-iku+s)^2$$

$$+ \int_o^{\infty} dv'\hat{h}_o(v').\ \int_o^{v'} du/(z(u)+iku+s)^2$$

(using (5.64).)

$$= \frac{\pi^{\frac{1}{2}}}{2}.\left\{\int_o^{\infty} du/(z(u)+iku+s)^2 + \int_o^{\infty} du/(z(u)-iku+s)^2\right\}$$

$$+ \frac{ik.}{2}\left\{\int_o^{\infty} du/(z(u)+iku+s)^2 - \int_o^{\infty} du/(z(u)-iku+s)^2\right\}$$

$$- 1/(1+s) \qquad (5.71)$$

By substituting I_b in equation (5.69) we obtain

$$ikA(s,k) = -\alpha_3 . B(s,k) \qquad (5.72)$$

where

$$\alpha_3 = \frac{\pi^{\frac{1}{2}}}{2} . \left\{ \int_0^\infty du/(z(u)+iku+s)^2 + \int_0^\infty du/(z(u)-iku+s)^2 \right\}$$

$$+ \frac{ik}{2} \left\{ \int_0^\infty du/(z(u)+iku+s)^2 - \int_0^\infty du/(z(u)-iku+s)^2 \right\} \qquad (5.73)$$

By solving the simultaneous pair of equations (5.72) and (5.68) we obtain for the unknown functions

$$A(s,k) = \frac{1}{2\pi^{3/2}} . (\alpha_3/\alpha_4) \qquad (5.74)$$

$$B(s,k) = \frac{1}{2\pi^{3/2}} . (-ik/\alpha_4) \qquad (5.75)$$

where

$$\alpha_4 = s\alpha_3 - ik\alpha_1$$

$$= k^2/(k^2 + \pi) + \frac{\pi^{\frac{1}{2}} s}{2} \left\{ \int_0^\infty du/(z(u)+iku+s)^2 \right.$$

$$\left. + \int_0^\infty du/(z(u)-iku+s)^2 \right\} \qquad (5.76)$$

Therefore,

$$f(k,v,s) = (1/2\pi^{3/2}).\left[\ \alpha_3/\alpha_4 - (ik/\alpha_4).\int_0^v du/(z(u)+iku+s)^2\ \right] \qquad (5.77)$$

For our purposes $Q(k,s)$ is the most important function and can easily be obtained from the above equation:

$$Q(k,s) = \int_{-\infty}^{\infty} dv\, h(k,v,s)$$

$$= \int_{-\infty}^{\infty} dv\, \hat{h}_0(v).f(k,v,s)$$

$$= (\alpha_3/2\pi\alpha_4) - (ik/2\pi^{3/2}\alpha_4).\ \alpha_5 \qquad (5.78)$$

where

$$\alpha_5 = \int_{-\infty}^{\infty} dv\, \hat{h}_0(v).\int_0^v du/(z(u)+iku+s)^2 \qquad (5.79)$$

(using (5.64).)

$$= \frac{\pi^{\frac{1}{2}}}{2}\left[\int_0^{\infty} du/(z(u)+iku+s)^2 - \int_0^{\infty} du/(z(u)-iku+s)^2\right]$$

$$+ \frac{ik}{2}\left[\int_0^{\infty} du/(z(u)+iku+s)^2 + \int_0^{\infty} du/(z(u)-iku+s)^2\right] \qquad (5.80)$$

By substituting the expression for α_5 in (5.78) we obtain by a simple calculation

$$Q(k,s) = \frac{(\pi+k^2).\, y(k,s)}{(\pi^{\frac{1}{2}} s y(k,s) + 2k^2/(k^2+\pi))} \cdot \frac{1}{(2\pi^{3/2})} \qquad (5.81)$$

where

$$y(k,s) = \int_{-\infty}^{\infty} \frac{du}{(z(u)+iku+s)^2} \qquad (5.82)$$

By using the above result for $Q(k,s)$ and equation (5.56) we can immediately obtain the explicit result for the differential energy cross section

$$S(k,\omega) = \frac{1}{2\pi^{3/2}} (\pi+k^2).\left[\frac{1}{(\pi^{\frac{1}{2}} i\omega y(k,i\omega) + 2k^2/(k^2+\pi))} \right.$$

$$\left. \frac{1}{(2k^2/(\pi+k^2) - i\omega\pi^{\frac{1}{2}} y(k,-i\omega))} \right]$$

(5.83)

where

$$y(k,\pm i\omega) = \int_{-\infty}^{\infty} \frac{du}{(z(u)+iku \pm i\omega)^2} \qquad (5.84)$$

Section 5.5. Spatial Moments and the Gaussian Approximation

The special Rayleigh model does not allow an analytic calculation of the Van Hove correlation function $G(x,\tau)$ as it does for $S(k,\omega)$, nevertheless, it does allow the analytic calculations of the spatial moments of $G(x,\tau)$ as a function of time. By analysing the Fourier-Laplace transform of $G(x,\tau)$ (which is given by $Q(k,s)$), it is quite simple to show the expected behaviour of $G(x,\tau)$. (see e.g. Lebowitz and Percus 1967.) However, it is much more convenient to consider the spatial moments which can be evaluated exactly by using $Q(k,s)$.

To do this calculation we note that

$$G(k,\tau) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx \exp(-ikx).G(x,\tau) \qquad (5.85)$$

and

$$Q(k,s) = \int_{o}^{\infty} d\tau \exp(-s\tau).G(k,\tau) \qquad (5.86)$$

Hence, $G(k,\tau)$ is a moment-generating function and

$$\langle x^n(s)\rangle = \pm 2\pi.\left(\frac{\partial^n}{\partial k^n} Q(k,s)\right)_{k=o} \qquad (5.87)$$

(+ if n/2 is even; - if n/2 is odd)

$\langle x^n(s)\rangle$ is the Laplace transform of the n^{th} spatial moment. All the odd spatial moments are zero because of the choise of the initial condition. The quantities of greatest

physical interest are the second and the fourth spatial moments. These are calculated below.

(a) The Second Spatial Moment

From (5.87) we have

$$\langle x^2(s)\rangle = -2\pi. \left[\frac{\partial^2}{\partial k^2} Q(k,s)\right]_{k=o} \qquad (5.88)$$

By using the expression (5.81) for $Q(k,s)$ we have

$$\langle x^2(s)\rangle = \frac{2}{\pi^{3/2} s^2 Q(\infty,s)} - \frac{2}{\pi s} \qquad (5.87)$$

after lengthy but straightforward calculations. In the above expression, $Q(\infty,s)$ is the function defined by equation (4.48). In order to check the correctness of this result, we note that

$$D_o = \int_o^\infty d\tau\, S_x(\tau) \qquad (\text{see } (5.23).)$$

$$= \underset{\tau \longrightarrow \infty}{\text{Limit}} (1/2). \frac{\partial}{\partial \tau} \langle x^2(\tau)\rangle \qquad (5.88)$$

(see e.g. Desai and Nelkin 1966.)

where D_o , the diffusion constant was derived earlier (5.24). Using the derivative theorem for Laplace transforms

$$\hat{L}\left[\frac{\partial}{\partial\tau}\ \frac{\langle x^2(\tau)\rangle}{2}\right] = s.\ \frac{\langle x^2(s)\rangle}{2} \qquad (5.89)$$

and the limit theorem (see e.g. Churchill 1958.)

$$\underset{s\longrightarrow o}{\text{Limit}}\ sf(s) = \underset{\tau\longrightarrow\infty}{\text{Limit}}\ f(\tau) \qquad (5.90)$$

we have

$$D_o = \underset{s\longrightarrow o}{\text{Limit}}\ \frac{s^2.\ \langle x^2(s)\rangle}{2}$$

$$= \frac{1}{\pi^{3/2}} \cdot \frac{1}{\int_o^\infty du/z(u)^2} \qquad (5.91)$$

which is precisely the result derived earlier by using $S_x(\tau)$. The formula (5.87) for the second moment is in the form where the numerical Laplace transform method discussed earlier can be applied quite readily. Numerical computation of the second spatial moment is discussed at the end of this section.

By applying the method of finding inverse Laplace transforms, developed in chapter four (see Appendix D)

we have

$$\langle x^2(\tau)\rangle = (2/\pi^{3/2}).\ \hat{L}^{-1}\left(1/s^2Q(\infty,s)\right)$$

$$- (2/\pi).\ \hat{L}^{-1}(1/s) \qquad (5.92)$$

But

$$L^{-1}\left(1/s^2Q(\infty,s)\right) = (1/2\pi i).\int_{\sigma-i\infty}^{\sigma+i\infty} ds\exp(s\tau)/s^2Q(\infty,s)$$

$$\sigma > 0$$

$$(5.93)$$

(see the contour diagram: Figure 15). The s^2 term in the integrand will give a contribution and therefore

$$\hat{L}^{-1}\left(1/s^2Q(\infty,s)\right) = a_1 - (1/2\pi i).\int_{CDEF} ds\exp(s\tau)/s^2Q(\infty,s)$$

$$(5.94)$$

where

a_1 = residue of $(1/s^2Q(\infty,s)).\exp(s\tau)$ at $s=o$

$$= \underset{s\longrightarrow o}{\text{Limit}}\ \frac{d}{ds}\left[s^2.\ \exp(s\tau)/s^2Q(\infty,s)\right]$$

$$= \tau/Q(\infty,o) + (2/Q(\infty,o)^2).\int_o^\infty du/z(y)^3$$

$$(5.95)$$

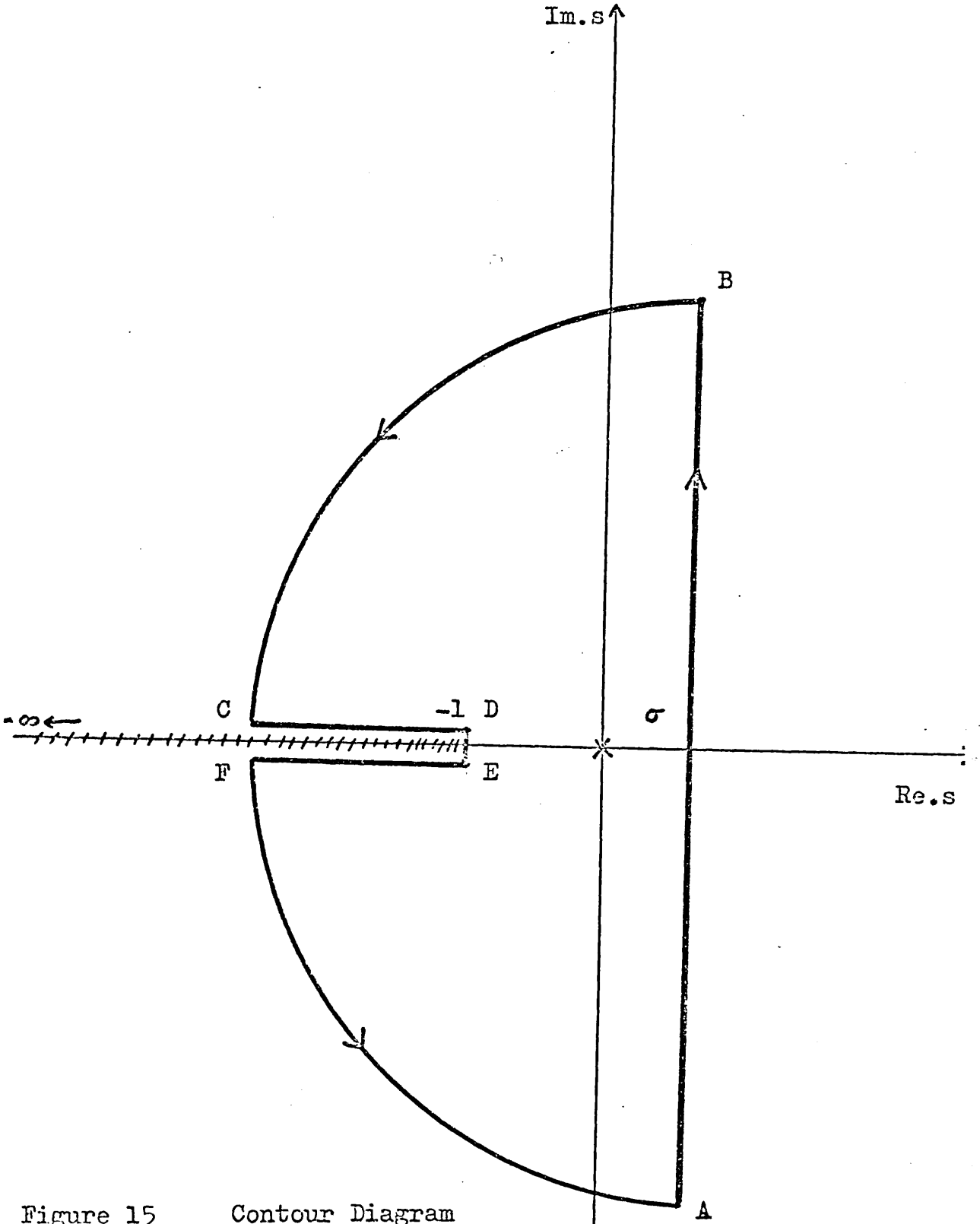


Figure 15 Contour Diagram for finding the inverse transforms of $\langle x^2(s) \rangle$ and $\langle x^4(s) \rangle$. The dashed line is the branch-cut and the pole is marked by a cross.

Along the branch cut the contour integral becomes

$$-(1/2\pi i).\int_{CDEF} ds\exp(s\tau)/s^2Q(\infty,s)$$

$$= \int_0^\infty \frac{dx_\lambda z'(x_\lambda)\exp(-z(x_\lambda)\tau).2iIm(\ B^-(\lambda)\ )}{2\pi i} \qquad (5.96)$$

where

$$2iIm(\ B^-(\lambda)\ ) = \text{Limit}_{\varepsilon \longrightarrow 0} \frac{1}{(-z(x_\lambda)-i\varepsilon)^2Q(\infty,-\lambda-i\varepsilon)}$$

$$- \frac{1}{(-z(x_\lambda)+i\varepsilon)^2Q(\infty,-\lambda+i\varepsilon)}$$

$$= \frac{2\pi i.g(\infty,\lambda)}{(\ R(\infty,\lambda)^2 + \pi^2 g(\infty,\lambda)^2\ ).z(x_\lambda)^2} \qquad (5.97)$$

Therefore,

$$\langle x^2(\tau)\rangle = 2D_o\tau + \left(4\pi^{3/2}D_o^2.\int_o^\infty du/z(u)^3 - 2/\pi\right)$$

$$+ (2/\pi^{3/2}).\int_0^\infty \frac{dx_\lambda z'(x_\lambda)\ g(\infty,\lambda)\exp(-z(x_\lambda)\tau)}{z(x_\lambda)^2.(\ R(\infty,\lambda)^2+\pi^2 g(\infty,\lambda)^2)} \qquad (5.98)$$

The third term on the right-hand side of equation (5.98) clearly shows the non-Gaussian behaviour of the second spatial moment in the intermediate-time regime. The asymptotic result $2D_o\tau$ is self-evident.

(b) The Fourth Spatial Moment

If the Gaussian description for $G(x,\tau)$, as first introduced by Vineyard (1958), applied to the special Rayleigh model then we could write

$$G(x,\tau) = (\pi\omega(\tau)^2)^{-\frac{1}{2}} . \exp(-x^2/\omega(\tau)^2) \qquad (5.99a)$$

so that

$$\frac{1}{3} . \frac{\langle x^4(\tau)\rangle}{\langle x^2(\tau)\rangle^2} = 1 \qquad (5.99b)$$

for all times. Therefore, to compare our analytic calculations with the Gaussian approximation, we can calculate the above ratio of moments to see possible deviations from unity.

Laplace transform of the fourth spatial moment is given by

$$\langle x^4(s)\rangle = + 2\pi . \left(\frac{\partial^4}{\partial k^4} Q(k,s) \right)_{k=o} \qquad (5.100)$$

After lengthy but quite straightforward calculations , the explicit expression for the transform of the moment follows as

$$\langle x^4(s)\rangle = \frac{24}{Q(\infty,s)^2 s^2 \pi^{3/2}} \left[\frac{1}{s.\pi^{3/2}} - 3 \cdot \int_0^\infty \frac{du \quad u^2}{(\, z(u) + s \,)^4} \right]$$

(5.101)

which can be simplified by using the identity

$$\int_0^\infty du \, \frac{u^2(z(u)-uz'(u))}{(\, z(u) + s \,)^4} = \frac{1}{3\pi^{3/2}} - \int_0^\infty \frac{du \quad u^2}{(\, z(u) + s \,)^4}$$

(5.102)

(which can be proved by a simple integration by parts.)

$$\langle x^4(s)\rangle = \frac{72}{Q(\infty,s)^2 s^3 \pi^{3/2}} \cdot \int_0^\infty du \, \frac{u^2(\, z(u) - z'(u)u \,)}{(\, z(u) + s \,)^4}$$

(5.103)

In this form, it is self-evident that the limit theorem (see e.g. Churchill 1958.)

$$\underset{s \longrightarrow \infty}{\text{Limit}} \; s \langle x^4(s)\rangle = \underset{\tau \longrightarrow 0}{\text{Limit}} \langle x^4(\tau)\rangle = 0$$

(5.104)

holds for the fourth spatial moment. Although it is possible to find an analytic expression for the above moment, it suffices here, only to consider the long-time behaviour of

the moment so that numerical results can be checked.

From equation (5.103) we see that the contour diagram for finding the inverse transform of the fourth spatial moment would contain the usual branch cut along the negative real-axis and a third order pole at s=o in the complex plane. From our experience with the second spatial moment we know that the residue of the pole will give the most important contribution in the long time limit. Therefore,

$$\langle x^4(s)\rangle = a_2 - \int_{CDEF} ds \frac{\exp(s\tau).\ \langle x^4(s)\rangle}{2\pi i} \qquad (5.105)$$

where the integral on the right-hand side above is along the branch cut and

$$a_2 = \underset{s \longrightarrow o}{\text{Limit}} \frac{1}{2}.\frac{d^2}{ds^2}\left[s^3 \exp(s\tau).\langle x^4(s)\rangle\right]$$

$$= \tau^2.\frac{(\langle x^4(s)\rangle)_{s=o}}{2} + \frac{\tau}{2}.\left(\frac{d}{ds}\langle x^4(s)\rangle\right)_{s=o} + \frac{1}{2}.\left(\frac{d^2}{ds^2}\langle x^4(s)\rangle\right)_{s=o} \qquad (5.106)$$

But

$$\left(\langle x^4(s)\rangle\right)_{s=o} = 24.D_o^2 \qquad (5.107a)$$

$$\left(\frac{d\langle x^4(s)\rangle}{ds}\right)_{s=o} = 72.D_o^2.\pi^{3/2}.\left[(4D_o/3).\int_o^\infty du/z(u)^3 - \int_o^\infty du\, u^2/z(u)^4\right] \qquad (5.107b)$$

and

$$\left(\frac{d^2}{ds^2}\langle x^4(s)\rangle\right)_{s=o} = 72.\left\{D_o^4.\pi \int_o^\infty du/z(u)^3 - 4.D_o^3.\pi^{3/2}\int_o^\infty du/z(u)^4 - \frac{8.(D_o\pi^{3/2})^3}{\pi^{3/2}}\int_o^\infty du/z(u)^3.\int_o^\infty du\, u^2/z(u)^4 + 8.(D_o^2.\pi^{3/2}).\int_o^\infty du\, u^2/z(u)^5\right\} \qquad (5.107c)$$

Finally,

$$a_2 = 12.D_o^2.\tau^2 + 12.D_o^2.\pi^{3/2}.\tau\left\{4.D_o.\left[\int_o^\infty du/z(u)^3\right] - 3.\left[\int_o^\infty du\, u^2/z(u)^4\right]\right\} + C_o \qquad (5.108)$$

where C_o is a constant and equal to $1/2.\left[\frac{d^2}{ds^2}\langle x^4(s)\rangle\right]_{s=o}$.

Therefore, the long-time behaviour of the

fourth spatial moment is of the form

$$\langle x^4(\tau)\rangle \underset{\tau\sim\infty}{\approx} 12.D_o^2.\tau^2 + C_1.\tau + C_o \qquad (5.109)$$

where C_1 is a constant.

(c) Numerical Computations

The numerical method of finding Laplace transforms has already been considered in this chapter. For the second and the fourth spatial moments the asymptotic results prove to be useful checks for the numerical validity of the results. We shall consider the Maxwellian heat-bath and therefore, $z(x) = \exp(-x^2) + \pi^{\frac{1}{2}}x\mathrm{erf}(x)$.

(i) Figure 16 shows the time evolution of the second spatial moment. The dashed line is the asymptotic result $2D_o\tau$ which is seen to be a very good approximation in the long time regime. The non-Gaussian behaviour in the intermediate time regime is quite evident.

(ii) Figure 17 shows the time evolution of the fourth spatial moment. The dashed line is the asymptotic result (5.109) where the numerical constants are:

$$\begin{aligned} D_o &= 0.185165. \\ C_1 &= -0.266276 \\ C_o &= 1.477456 \end{aligned} \qquad (5.110)$$

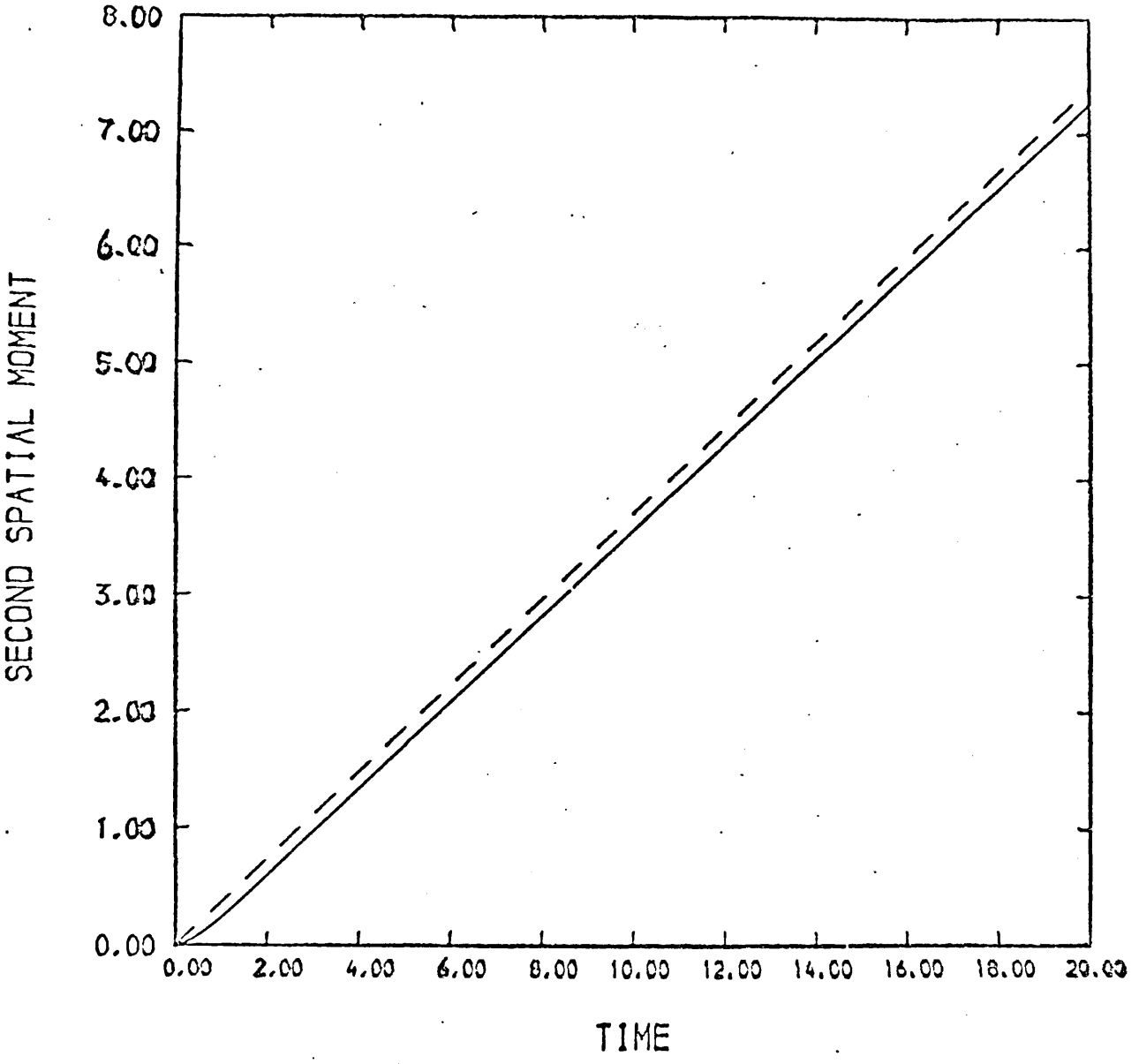


Figure 16: The Time Evolution Of The Second Spatial Moment. The dashed line represents the aymptotic result $2D_o\tau$.

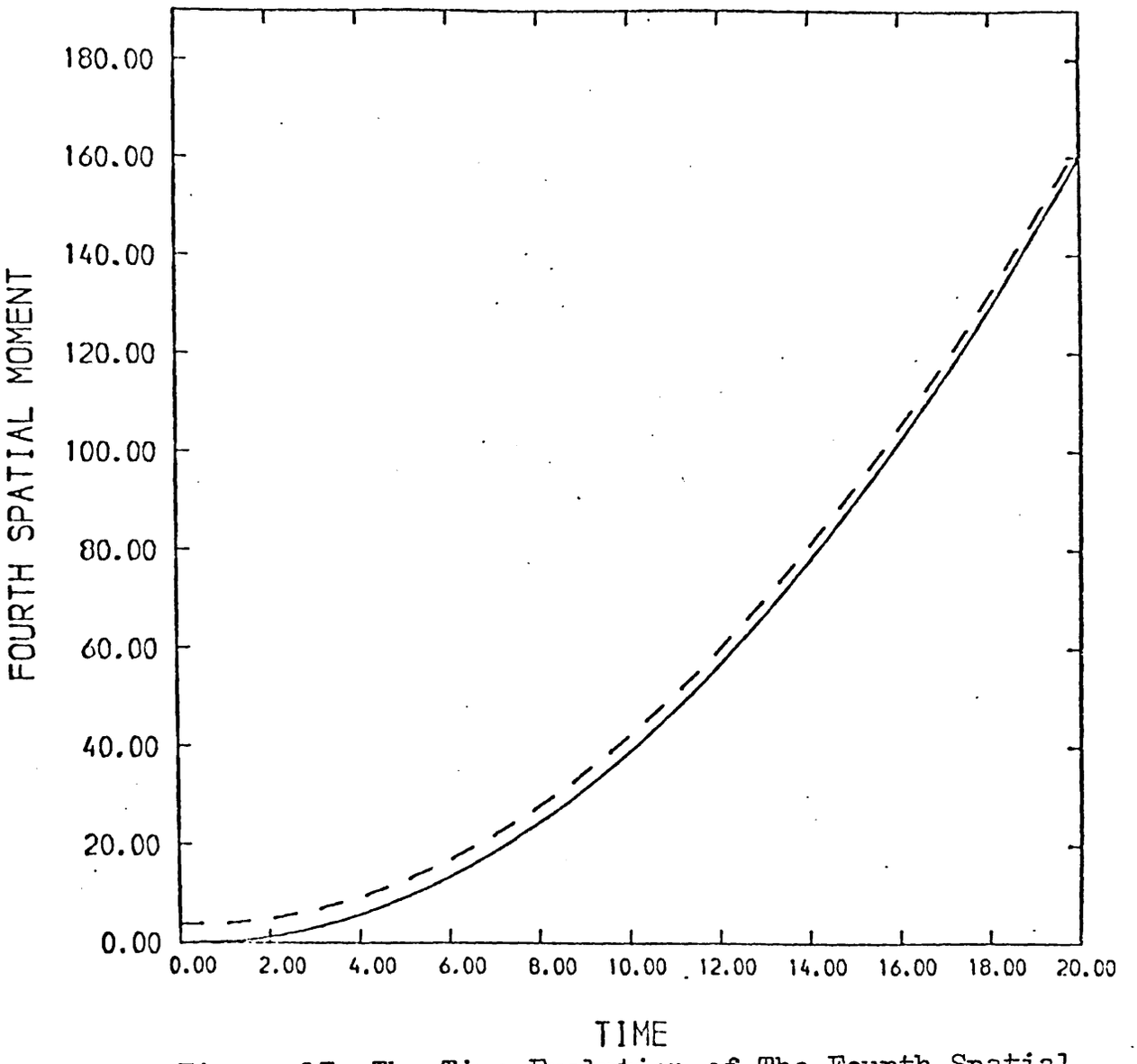


Figure 17 The Time Evolution of The Fourth Spatial Moment. The dashed curve is the aymptotic result (5.109).

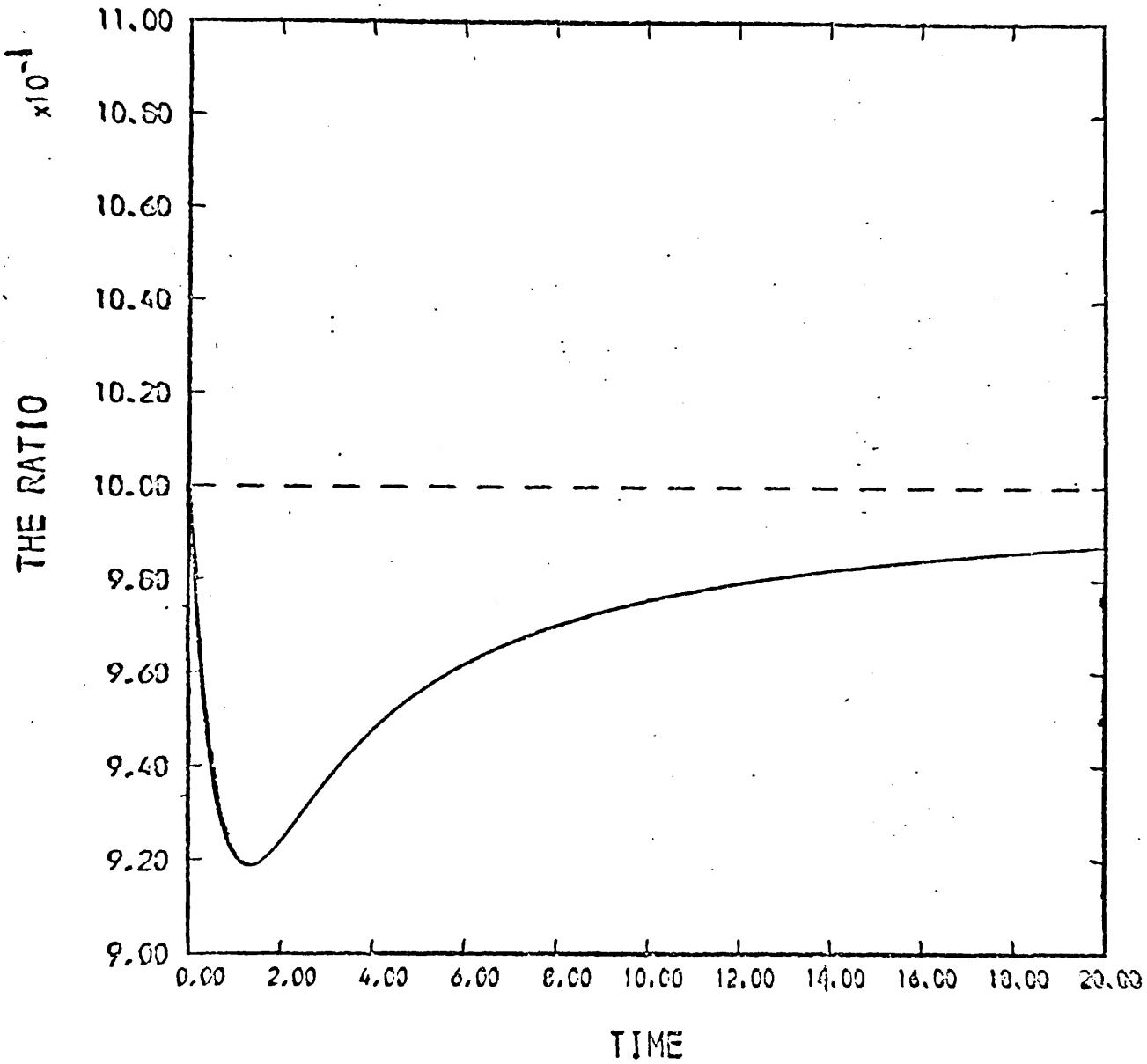


Figure 18 The Ratio of Moments (for the Gaussian distribution, the ratio would be equal to unity at all times.). Notice the convergence to Gaussian behaviour at long times and near the origin.

(iii) Figure 18 shows the time evolution of the ratio:

$$\left(\frac{\langle x^4(\tau) \rangle}{3.(\langle x^2(\tau) \rangle)^2} \right)^{-1}$$

which for the Gaussian approximation is exactly one. We see that the approximation holds for the special Rayleigh model in the limit of short and long times, but not at intermediate times. The ratio reaches the minimum of about 0.9 after roughly one collision-time in the scaled units. After about three units of scaled time the ratio is practically identical to unity as one would expect from the asymptotic results for the moments. Nonetheless, the approximation is clearly a poor one in terms of the result at all times, which is hardly surprising when one considers the important contribution made by integrals along the branch cut.

(* Just before the publication of this thesis, it came to the knowledge of the author that P. Resibois (Physica 90A, p.273 (1978).) has quite independently arrived at the solution of the spatial problem. However, Resibois was not able to give explicit expression for the autocorrelation function and the second spatial moment nor did he obtain the ratio of moments.)

APPENDIX A

(a) Approach to Equlibrium

We shall show that any time dependent solution of the Master equation (1.16) tends to $P_{eq}(x)$ or

$$\lim_{t \to 0} P(x,t) = P_{eq}(x)$$

Consider an arbitrary non-negative convex function $f(q)$:

$$f(q) \geq 0 \qquad \text{for} \qquad 0 < q < \infty,$$

$$f(q) > 0 \qquad \text{for} \qquad 0 < q < \infty.$$

Define

$$H(t) = \int dx\, P_{eq}(x) f\,(q(x,t)) \qquad (A.1)$$

where

$$q(x,t) = P(x,t)/P_{eq}(x) \qquad (A.2)$$

From (1.16) and using the detailed balance condition we have,

$$\frac{dH(t)}{dt} = \int dx \frac{\partial}{\partial q} f(q) . \frac{\partial}{\partial t} P(x,t)$$

$$= \iint dx dx' K(x|x') P_{eq}(x') . \Big[q(x',t) \frac{\partial}{\partial q} f(q(x,t)) - q(x',t) . \frac{\partial}{\partial q'} f(q(x',t)) \Big] \qquad (A.3)$$

by rearranging and relabelling. For an arbitrary $\rho(x)$ one easily sees that

$$0 = \iint dxdx' k(x|x') P_{eq}(x'). \left[\rho(x) - \rho(x') \right] \qquad (A.4)$$

If one chooses $\rho(x) = f(q(x,t)) - q(x,t).\frac{\partial}{\partial q} f(q(x,t))$

and add the identity obtained to $H'(t)$ above then one obtains

$$H'(t) = \iint dxdx' P_{eq}(x') k(x|x') \Big\{ \left[q(x',t) - q(x,t) \right] . \frac{\partial}{\partial q} f(q) + f(q(x,t)) - f(q(x',t)) \Big\} \qquad (A.5)$$

Now for any convex function $f(q)$ the term in the integrand above within the square brackets is negative unless $q(x,t) = q(x',t)$. ($f(q) + (q-q').f'(q) \leqslant f(q')$.)

Hence $H(t)$ decreases in time and must therefore approach a limit. In this limit one must have $H'(t) = 0$. or

$\underset{t \to \infty}{\text{Limit}}\ P(x,t)/P_{eq}(x)$ = constant. Because of normalisation, the constant must equal to one. Q.E.D.

(b) The operator $\hat{A}$ is negative semi-definite

The operator $\hat{A}$ is negative semi-definite with the consequence

that the eigenvalues must be positive.

Consider the inner product or the matrix element

$$(f, \hat{A}f) = \int f(x) . \int G(x|y)f(y)dydx - \int A(x)f(x)^2 dx$$

$$= \int f(x)\left[\int \left(G(x|y)f(y) - G(x|y)\frac{N(y)}{N(x)}f(x) \right)dy \right]dx$$

$$= -\frac{1}{2}\iint G(x|y)N(x)N(y)\left\{ f(x)/N(x) - f(y)/N(y) \right\}^2 \qquad (A.6)$$

The last steps follows by using the property

$G(x|y) = G(y|x)$ and the identity

$$\iint dxdy\, G(x|y)N(y)\frac{f(x)^2}{N(x)} = \iint G(y|x)\frac{N(x)}{N(y)}f(y)^2 dxdy \qquad (A.7)$$

Therefore,

$$(f, \hat{A}f) \leq 0. \quad \text{Q.E.D.}$$

APPENDIX B

The Collision Number Function Z(V) For the Rayleigh Model

$$K(V|V') = \mu^2 C\,|V-V'|\,(m/2\pi kT)^{\frac{1}{2}} \exp\left(-\frac{m}{2kT}\left[(V'-V).\mu + V\right]^2\right) \qquad (B.1)$$

and

$$Z(V) = \int_{-\infty}^{\infty} dV' K(V|V') \qquad (B.2)$$

By making the change of variables (2.14) we have,

$$Z(V) = C.(2kT/m)^{\frac{1}{2}}.\mu^2 \int_{-\infty}^{\infty} dy\,|x-y|\,e^{-((y-x).\mu + x)^2} \qquad (B.3)$$

But

$$z(x) = \mu^2 \cdot \int_{-\infty}^{\infty} dy\,|x-y|\,e^{-((y-x).\mu + x)^2}$$

$$= \mu^2 \cdot \left\{ \int_0^{\infty} dt\, t \exp(-[x+t.\mu]^2) + \int_0^{\infty} t \exp(-[x-\mu t]^2)\,dt \right\}$$

$$= \int_x^{\infty} dy(y-x)e^{-y^2} + \int_{-\infty}^{x} dy(x-y)e^{-y^2}$$

$$= \pi^{\frac{1}{2}} x\,\mathrm{erf}(x) + e^{-x^2} \qquad (B.4)$$

Therefore,

$$Z(V) = C\,V.\mathrm{erf}\left((m/2kT)^{\frac{1}{2}}.V\right) + (2kT/\pi m)^{\frac{1}{2}}.\exp(-mV^2/2kT).C \qquad (B.5)$$

APPENDIX C

C.1. The Pseudofunction $R(x,\lambda)$

Hoare and Rahman have discussed in detail the properties of the above pseudofunction. Technically, one ought to understand $R(x,\lambda)$ by the following definition:

$$\langle Pf.R(x,\lambda),\ \phi(x)\rangle = Fp.\int_{-\infty}^{\infty} R(x,\lambda)\phi(x)dx \qquad (C.1)$$

Without the complications of distribution theory, it is possible to resolve $R(x,\lambda)$ into its regular and singular components by making a Taylor series expansion of $(z(y)-\lambda)$ about the point $y=x_\lambda$:

$$R(x,\lambda) = \int_0^{x} dy/(z(y)-z(x_\lambda))^2$$

$$= \mathrm{sgn}(x)\int_0^{|x|}\left(1/(z(y)-z(x_\lambda))^2 - 1/z'(x_\lambda)^2(y-x_\lambda)^2\right)dy$$

$$+ \frac{\mathrm{sgn}(x)}{z'(x_\lambda)^2}\left[\frac{1}{|x|-|x_\lambda|} + \frac{1}{|x_\lambda|}\right] \qquad (C.2)$$

Essentially in this form, only Cauchy-Principal values have to be considered.

C.2. Orthogonal Integrals

$$I_1 = \int_{-\infty}^{\infty} dx\hat{h}_o(x)\phi_{ev}(x,\lambda)\phi_{ev}(x,\lambda') \qquad (C.3)$$

We shall require the following identities:

(a) $$[H(x-|x_\lambda|)-H(x+|x_\lambda|)].[\delta(x-|x'_\lambda|)+\delta(x+|x'_\lambda|)]$$

$$= \delta(x-|x'_\lambda|)+\delta(x+|x'_\lambda|) \qquad (C.4)$$

(b) $$(H(x-|x'_\lambda|)-H(x+|x'_\lambda|)).(\delta(x-|x_\lambda|)+\delta(x+|x_\lambda|)) = 0 \qquad (C.5)$$

(c) $$\{H(x-|x_\lambda|)-H(x+|x_\lambda|)\}.\{H(x-|x'_\lambda|)-H(x+|x'_\lambda|)\}$$

$$= H(x-|x'_\lambda|)-H(x+|x'_\lambda|) \qquad (C.6)$$

Therefore by substituting the expression (3.82) for $\phi_{ev}(x,\lambda)$ and using the above identities it follows that

$$I_1 = A(\lambda)A(\lambda').\Big(-2\int_0^{|x'_\lambda|}\hat{h}_o(x)dx + 2q(x'_\lambda)\hat{h}_o(x'_\lambda) + 2q(x'_\lambda)q(x_\lambda)\hat{h}_o(x_\lambda).\delta(|x_\lambda|-|x'_\lambda|)\Big)$$

$$= \frac{z'(|x_\lambda|)^3}{z''(x_\lambda)}.A(\lambda)^2.\delta(\lambda-\lambda') \qquad (C.7)$$

$$I_2 = \int_{-\infty}^{\infty} dx\hat{h}_o(x)\phi_{od}(x,\lambda)\phi_{od}(x,\lambda') \qquad (C.8)$$

We shall require the identities:

$$(a)\quad \{H(x-|x_\lambda|) - H(-x-|x_\lambda|)\} \cdot \{\delta(x-|x'_\lambda|) - \delta(x+|x'_\lambda|)$$

$$= 0 \qquad (C.9)$$

$$(b)\quad \{H(x-|x'_\lambda|)-H(-x-|x'_\lambda|)\} \cdot \{\delta(x-|x_\lambda|)-\delta(x+|x_\lambda|)\}$$

$$= \delta(x-|x_\lambda|) - \delta(x+|x_\lambda|) \qquad (C.10)$$

$$(c)\quad \{H(x-|x'_\lambda|)-H(-x-|x'_\lambda|)\} \cdot \{H(x-|x_\lambda|)-H(-x-|x_\lambda|)\}$$

$$= H(x-|x_\lambda|)-H(-x-|x_\lambda|) \qquad (C.11)$$

Let $J_2 = \left(R(x,\lambda)-R(\infty,\lambda).g(x,\lambda)\right) \cdot \left(R(x,\lambda')-R(\infty,\lambda').g(x,\lambda')\right)$

By using the relationships:

$$2\int_0^\infty dy R(y,\lambda)R(y,\lambda')\hat{h}_o(y) = \pi^{\frac{1}{2}}R(\infty,\lambda)R(\infty,\lambda') - \left(\frac{R(\infty,\lambda)-R(\infty,\lambda')}{\lambda-\lambda'}\right) \qquad (C.12)$$

and

$$2\int_0^\infty dy \hat{h}_o(y)R(y,\lambda') = \pi^{\frac{1}{2}}R(\infty,\lambda')-z'(|x_\lambda|)R(|x_\lambda|,\lambda') - 1/(\lambda-\lambda') \qquad (C.13)$$

the required integral becomes:

$$I_2 = A_2(\lambda)A_2(\lambda').\int_{-\infty}^{\infty} dy\ J_2.\hat{h}_o(y)$$

$$= A_2(\lambda)^2.\ R(\infty,\lambda)^2 \frac{z'(|x_\lambda|)^3}{z''(x_\lambda)}\ \delta(\lambda-\lambda') \qquad (\ C.14\ )$$

(Where the identities (C.9) to (C.11) have been used.)

Finally,

$$I_3 = \int_{-\infty}^{\infty} dx \hat{h}_o(x)\phi_{ev}(x,\lambda)$$

$$= A(\lambda).\left[\ 2\int_{0}^{|x_\lambda|} dy \hat{h}_o(y)\ -\ z'(|x_\lambda|)\right]$$

$$= 0. \qquad (\ C.15\ )$$

where we have used the expression (3.82) for the even eigendistribution.

APPENDIX D

D.1 The Rigorous Proof of the Relationship:

$$L^{-1}\,Q(x,s) = \tau\int_0^{\infty} dy \exp(-z(y)\tau) \qquad (\text{D.1})$$

By definition,

$$L^{-1}Q(x,s) = \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds \exp(s\tau).Q(x,s) \qquad (\text{D.2})$$

If we integrate $Q(x,s)$ around the contour ABCDEF then from Cauchy theorem it follows that

$$\oint_C ds Q(x,s)e^{s\tau} = 0 \qquad (\text{D.3})$$

But,

$$\oint_C ds\, Q(x,s)e^{s\tau} = \int_{\sigma-iA}^{\sigma+iB} ds e^{s\tau}Q(x,s) + \int_{BC} ds e^{s\tau}Q(x,s) + \int_{CDEF} ds e^{s\tau}Q(x,s) + \int_{FA} ds e^{s\tau}\,Q(x,s) \qquad (\text{D.4})$$

The first integral on the right-hand side approaches $L^{-1}Q(x,s)$ as A and B are made to approach -oo and +oo respectively. In this limit, portions BC and FA contribute nothing, because of the rapid decrease of $\exp(s\tau)$.

Therefore,

$$\int_{\sigma-i\infty}^{\sigma+i\infty} ds\exp(s\tau)Q(x,s) = -\int_{CDEF} ds\exp(s\tau)Q(x,s) \qquad (\text{D.5})$$

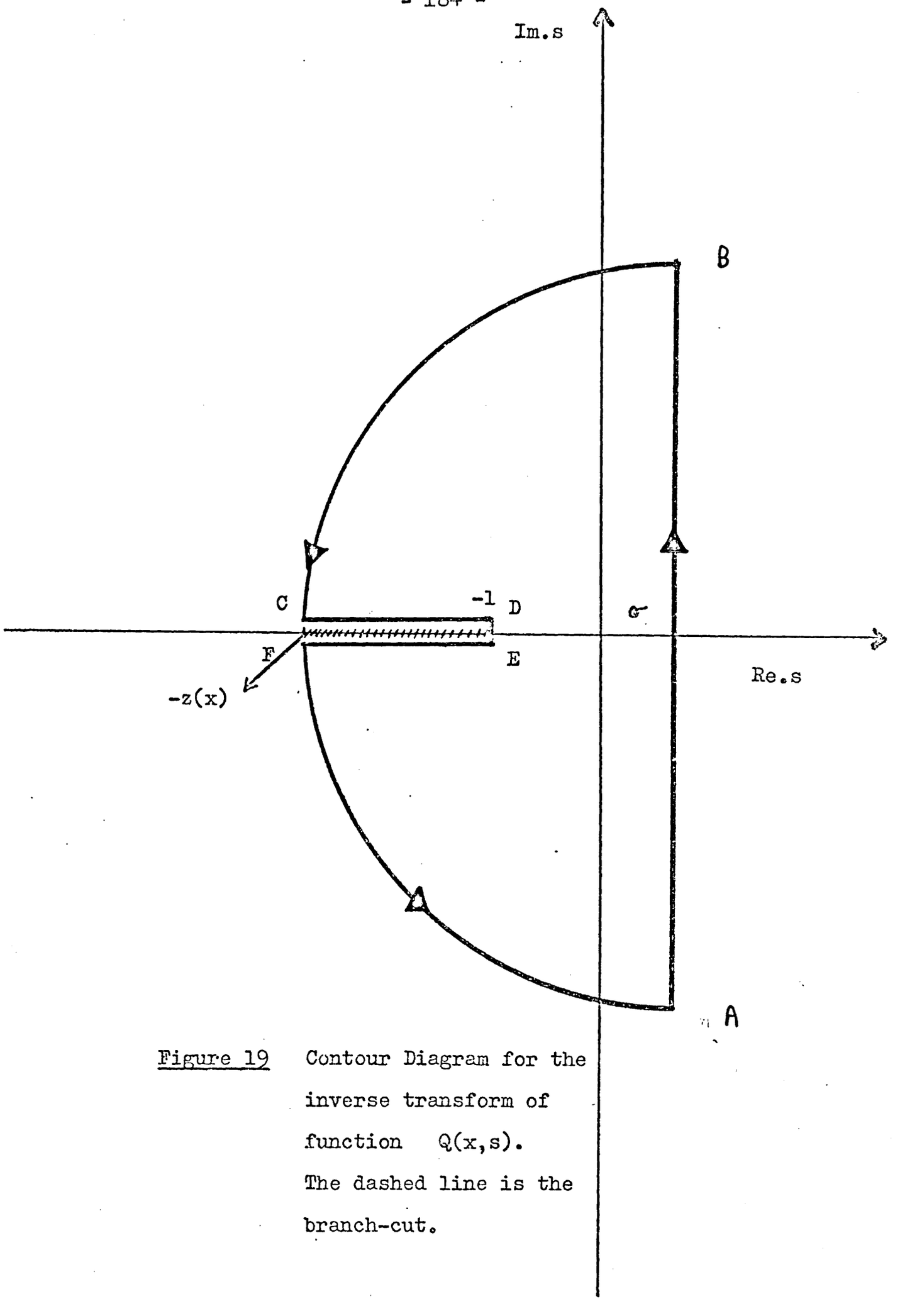


Figure 19 Contour Diagram for the inverse transform of function Q(x,s). The dashed line is the branch-cut.

Along lines CD and EF we can evaluate the integrals as follows. Note that the integral over a small semicircle of radius ε centred at -1 vanishes as ε tends to zero (same is true in case of a semicircle about $s=-z(x)$). $Q(x,s)$ is analytic in the the whole complex plane except along the line from -1 to $-z(x)$.

Next we shall bring the lines CD and EF close to the real axis, an operation performed by letting $\varepsilon \longrightarrow o$ where $s=-\lambda \pm i\varepsilon$.

$$L^{-1}Q(x,s) = \frac{1}{2\pi i} \int_{z(o)}^{z(x)} d\lambda e^{-\lambda\tau} \{Q^-(\lambda)-Q^+(\lambda)\} \qquad (D.6)$$

where,

$$\{Q^-(\lambda)-Q^+(\lambda)\} = \underset{\varepsilon \to o}{\text{Limit}} \{Q(x,-\lambda-i\varepsilon)-Q(x,-\lambda+i\varepsilon)\}$$

$$= 2i\,\text{Im}\, Q^-(\lambda) \qquad (D.7)$$

By using the identity (see e.g. Jones 1966)

$$\underset{\varepsilon \to o}{\text{Limit}} \frac{1}{(z(x)-\lambda \pm i\varepsilon)^2} = \text{Pf.}\frac{1}{(z(x)-\lambda)^2} \pm \delta'(z(x)-\lambda) \qquad (D.8a)$$

we have,

$$\underset{\varepsilon \to o}{\text{Limit}}\, Q(x,-\lambda \pm i\varepsilon) = R(x,\lambda) \pm i\pi \int_o^x du\,\delta'(z(u)-\lambda) \qquad (D.8b)$$

It can be shown that

$$\int_0^{x} \delta'(z(u)-\lambda)du \;=\; g(x,\lambda) \qquad (\text{D.9})$$

$g(x,\lambda)$ was defined in equation (3.119). Therefore,

$$Q^{+}(\lambda) = R(x,\lambda) + i\pi g(x,\lambda) \qquad (\text{D.10a})$$

$$Q^{-}(\lambda) = R(x,\lambda) - i\pi g(x,\lambda) \qquad (\text{D.10b})$$

and

$$2i\,\mathrm{Im}Q^{-}(\lambda) = -2\pi i g(x,\lambda). \qquad (\text{D.10c})$$

Finally,

$$\begin{aligned} L^{-1}Q(x,s) &= -\int_0^{|x|} dx_\lambda e^{-z(x_\lambda)\tau}\left(z'(x_\lambda)g(x,x_\lambda)\right) \\ &\equiv -\int_0^{|x|} dx_\lambda\; z''(x_\lambda)/z'(x_\lambda)^2 .\; \left[H(x-|x_\lambda|)-H(-x-|x_\lambda|)\right] \\ &\qquad \cdot e^{-z(x_\lambda)\tau} \\ &\quad - \int_0^{|x|} dx_\lambda \frac{e^{-z(x_\lambda)\tau}}{z'(x_\lambda)} .\; \left(\delta(x-|x_\lambda|)-\delta(x+|x_\lambda|)\right) \end{aligned} \qquad (\text{D.11})$$

Using the relationship:

$$\begin{aligned} &\int_0^{|x|} d\left(1/z'(x_\lambda)\right) \quad \exp(-z(x_\lambda)\tau).\left[H(x-|x_\lambda|)-H(-x-|x_\lambda|)\right] \\ &\qquad = \tau\int_0^{x} dy \exp(-z(y)\tau) + \int_0^{|x|} dx_\lambda \frac{e^{-z(x_\lambda)\tau}}{z'(x_\lambda)}\left(\delta(x-|x_\lambda|)\right. \\ &\qquad\qquad \left. -\delta(x+|x_\lambda|)\right) \end{aligned} \qquad (\text{D.12})$$

It follows that

$$L^{-1}Q(x,s) = -\tau\int_0^x du\exp(-z(u)\tau) \qquad (D.13)$$

Q.E.D.

D.2 Proof of the relationship

$$J_1 = \int_0^\infty dx_\lambda z'(x_\lambda)\exp(-z(x_\lambda)\tau).\frac{g(x,\lambda)g(x_o,\lambda)}{g(\infty,\lambda)}$$

$$= -\operatorname{sgn}(x)\operatorname{sgn}(x_o).\tau\int_0^{\min(|x|,|x_o|)} du e^{-z(u)\tau} + \frac{e^{-z(x_o)\tau}P_{od}(x,o)}{\hat{h}_o(x)} \qquad (D.14)$$

By substituting $g(x,\lambda)$ etc. in the above expression, we have

$$J_1 = D_1 + D_2 + D_3 \qquad (D.15)$$

where

$$D_1 = \int_0^\infty d(-1/z'(x_\lambda))e^{-z(x_\lambda)\tau}.\left(H(x-|x_\lambda|)-H(-x-|x_\lambda|)\right).\left(H(x_o-|x_\lambda|)-H(-x_o-|x_\lambda|)\right) \qquad (D.16)$$

$$D_2 = \int_0^\infty dx_\lambda \frac{\exp(-z(x_\lambda)\tau)}{z'(x_\lambda)}\left[H(x-|x_\lambda|)-H(-x-|x_\lambda|)\right].\left[\delta(x_o-|x_\lambda|)-\delta(x_o+|x_\lambda|)\right]$$

$$+ \left[H(x_o-|x_\lambda|)-H(-x_o-|x_\lambda|)\right].\left[\delta(x-|x_\lambda|)-\delta(x+|x_\lambda|)\right] \qquad (D.17)$$

and

$$D_3 = \int_0^{\infty} \frac{dx_\lambda e^{-z(x_\lambda)\tau}}{z''(x_\lambda)} \left(\delta(x-|x_\lambda|)-\delta(x+|x_\lambda|)\right).\left(\delta(x_o-|x_\lambda|)\right.$$
$$\left.\delta(x_o+|x_\lambda|)\right) \qquad (D.18)$$

Now by integration by parts we can write D_1 as

$$D_1 = -\tau\,\mathrm{sgn}(x)\mathrm{sgn}(x_o)\int_0^{\min(|x|,|x_o|)} du e^{-z(u)\tau} - D_2 \qquad (D.19)$$

and

$$D_3 = \frac{\exp(-z(x_o)\tau).P_{od}(x,o)}{\hat{h}_o(x)} \qquad (D.20)$$

Therefore,

$$J_1 = -\mathrm{sgn}(x)\mathrm{sgn}(x_o)\tau\int_0^{Min(|x|,|x_o|)} du e^{-z(u)\tau} + \frac{e^{-z(x)\tau}P_{od}(x,o)}{\hat{h}_o(x)}$$

Q.E.D.

Bibliography

Akama. H. and Siegel. A. ; Physica 31 , p.1493 (1965)

---------- Phys.Fluids. 8 , p.1218 (1965)

Alkemade. C.T.J. ; Physica 24 , p.1029 (1956)

Balescu. R. ; "Equlibrium and Non-equlibrium Statistical Mechanics." John Wiley & Sons, 1975

Barker. J.A. ;et. al. ; Can.J.Phys. 55 , p.916 (1977)

Bartlett. M.S. ; "Essays on Probability Theory and Statistics." London, Methuen, 1962

Boltzmann. L. ; Wien.Ber.66 , p.275 (1872)

Bremermann. H. ; "Distributions, Complex Variables and Fourier Transforms." Addison-Wesley,Reading,Mass., 1965

Burke. J. ; Physics Bulletin , p.545 (December 1976)

Case. K.M. and Zweifel. P.F. ; " Linear Transport Theory." Addison-Wesley,Reading,Mass., 1967

Case. K.M. ; Ann.Phys. (N.Y.) 7, p.349 (1959)

---------- Ann.Phys. (N.Y.) 9, p.1 (1960)

Chandrasekhar. S. ; Rev.Mod.Phys. 15 , p.1 (1943)

Churchill. R.V.; " Operational Mathematics." Mc-Graw Hill, New York, 1958

Corngold. N. and Shapiro. C.S. ; Phys.Rev. 137A , p.1686 (1965)

Cox. D.R. and Miller. H.D.; "The Theory of Stochastic Processes" Methuen & Co., London, 1965

Crump. K.S ; J.Am. Soc.Comp.Manf. 23 ,p.89 (1976)

Cukier. R.I. and Hynes. J.T. ; J.Chem. Phys. 64 , p. 2674 (1976)

Desai. R.C and Nelkin. M. ; Nuclear Sci. and Eng. 24 , p.142 (1966)

Doetsch. G. ; " Introduction to the theory and application of the Laplace Transform (Translated by W. Nader)." Spriger-Verlag, Berlin, 1974

Dubner. H. and Abate. J. ; J.Am.Soc.Comp.Manf. 15 , p.115 (1968)

Durbin. F. ; Comput.J. 17 , p.371 (1974)

Einstein. A. ; " Investigations on the theory of the Brownian movement." New York, Dover, 1956 (Contains translations of Einstein's 1905 papers.)

Erdelyi. A. ; "Higher Transcendental Functions Vol.1-3." New York, Mc-Graw Hill, 1953

" Tables of Integral Transforms Vol.1,2." New York, Mc-Graw Hill, 1954

Felderhof. B.U. ; Ned.T.Natuurk. 27 , p.236 (1961)

Ford. G.W. et. al. ; J.M.Phys. 6 , p.504 (1965)

Frisch. H.L. ; Phys.Rev. 104 , p.1. (1956)

Green. M.S. ; J.Chem.Phys. 19 , p.1036 (1951)

Hagelbroek. R.J. ; Ph.D. Thesis, University of Groingen, 1973

Haken. H. ; Rev.Mod.Phys. 47 , p.67 (1975)

---------- " Synergetics:An Introduction." Berlin, Springer, 1977

Hoare. M.R. ; Adv.Chem.Phys. 20 , p.135 (1971)

Hoare. M.R. and Kaplinsky. C.H. ; J.Chem.Phys. 52 ,p.3336 (1971)

---------- Physica 81A ,p.349 (1975)

Hoare. M.R. and Rahman. M. ; J.Phys.A. 6 ,p.1461 (1973)

---------- J.Phys.A. 7 ,p.1070 (1974)

---------- J.Phys.A. 9 ,p.77 (1976)

Jepson. D.W. ; J.Math.Phys. 6 ,p.405 (1965)

Jones. D.S. ; "Generalised Functions" Mc-Graw Hill, London, 1966

Keilson. J. and Storer. J.E. , Q.Appl.Math. 10 ,p.243 (1952)

Kolmogorov. A,N, ; Math.Ann. 104 , p.415 (1931)

Koppel. J.U. ; Nuclear Sci. and Eng. 16 , p.101 (1963)

Köthe. K. ; Math.Zeitschrift. 57 , p.13 (1952)

Kramers. H.A. ; Physica. 7 , p.284 (1940)

Kubo. R. ; Proc.Phys.Soc.Japan. 12 ,p.570 (1958)

Kuščer. I. and Williams. M.M.R. ; Phys.Fluids. 10 , p.1922 (1967)

Larson. V.H. ; Int.J.Control. 9 , p. 709 (1969)

Lebowitz. J.L. and Bergmann. P.G. ; Ann.Phys. (N.Y.) 1 , p.1. (1957)

Lebowitz. J.L. and Percus. J.K. ; Phys.Rev.155 , p.122 (1967)

---------- Phys.Rev.171 , p.224 (1968)

Lighthill. M.J. ; " Introduction to Fourier Analysis and Generalised Functions." Cambridge University Press,London, 1958

Mika. J.R. ; Nuclear Sci.and Eng. 11 , p.415 (1961)

Moyal. J.E. ; J.Roy. Statist.Soc. B11 , p.150 (1949)

Muskhelishvili. N.I. ; " Singular Integral Equations." P. Nordhoff, Gronigen, 1953

Rahman. A. et. al. ; Phys.Rev. 126 , p.986 (1962)

Rayleigh, Lord. ; Philos.Mag. 32 , p.424 (1891)

---------- "Scientific Papers." Cambridge Univ.Press, London, 1902

Razavy. M. ; Physica 81A , p. 591 (1976)

Sato. M. ; J.Fac.Sci. Univ. Tokyo. Sect.1 8 , p.139 (1959)

--------- J,Fac,Sci. Univ. Tokyo. Sect.2 8 , p.387 (1960)

Schizuta. Y. ; Pror.Theoret.Phys. (kyoto) 32 , p.489 (1964)

Schwartz. L. ; "Mathematics for the Physical Sciences." Addison-Wesley, Reading, Mass., 1966

Schottky. W. ; Ann.der.Physik. 57 , p.541 (1918)

Siegel. A. ; J.Math.Phys. 1 , p.378 (1960)

Smoluchowski. M.V. ; Physik.Zeit. 17 , p.557 (1916)

Teramoto. E. and Suzuki. C. ; Prog.Theoret.Phys. (koyoto) 14 , p.411 (1955)

Tillman. H.G. ; Math.Zeitschrift. 77 , p.106 (1961)

Tricomi. F.G. ; "Integral Equations." Interscience, New York, 1957

Van Hove. L. ; Phys,Rev. 95 , p.249 (1954)

Van Kampen. N.G. ; Physica 21 , p.949 (1955)

---------- Physica 26 , p.585 (1960)

---------- Can.J. Phys. 39 , p.551 (1961)

Vineyard. G.H. ; Phys.Rev. 110 , p.999 (1958)

Waldmann. L. ; " Handbuch der Physik." S.Flugge, Ed., Vol.12, Springer,Berlin, 1958

Williams. M.M.R. ; " The slowing down and thermalisation of neutrons." North Holland, Amsterdam, 1966

---------- " Mathematical Methods in Particle Transport Theory." London, Butterworths, 1971

---------- Nuclear Sci. and Eng. 26 , p.262 (1966)

---------- Nuclear Sci, and Eng. 33 , p.262 (1968)

Wood. T. ; Proc.Phys.Soc. 85 , p.805 (1965)

Wynn. P. ; Math.Tables.Aids. Comps. 10 , p.91 (1956)

Zelazny. R. and Kuszell. A. ; Ann.Phys. (N.Y.) 16 , p.81 (1962)

Zemanian. A.H. ; "Distribution Theory and Transform Analysis." Mc-Graw Hill, London, 1965

B. Davison Montreal Report A.E.C.L. M.T.112 (1944)

SHANKS. D. J. Math Phys. 34 p.1 (1955).

PART II

Physica **82A** (1976) 151–162

DIAMAGNETISM OF A CONFINED ELECTRON GAS*

B.U. FELDERHOF

Institut für Theoretische Physik A, RWTH Aachen, 51 Aachen, Germany

and

S.P. RAVAL

Department of Physics, Bedford College, Regent's Park, London NW 1, England

Received 11 June 1975

We consider a free electron gas in the presence of a uniform magnetic field and confined by a cylindrically symmetric harmonic potential in the directions normal to the field. The density matrix in Boltzmann statistics is evaluated exactly and it is shown that the electron gas rotates uniformly under the influence of the field. The corresponding Wigner distribution function is also studied.

1. Introduction

As is well known the theory of diamagnetism of metals is complicated and abounds with subtle pitfalls[1]). One of the reasons is that in the calculation of the bulk susceptibility it is essential to take boundary effects into account. This was first clearly realized in the classical theory after Miss van Leeuwen formulated her famous theorem[2]), by which she dealt a fatal blow to some of the older theories of diamagnetism. According to this theorem, proposed independently by Bohr[3]), the current density vanishes and hence the magnetic moment is zero in classical systems of charged particles in thermal equilibrium in the presence of an external magnetic field. It was shown by Landau[4]) that this is not true in quantum mechanics and that in fact the diamagnetic susceptibility of an electron gas is just one third the paramagnetic susceptibility due to spin.

Landau evaluated the quantum partition function, using an interesting set of single particle wavefunctions, and taking proper care of the effects of the boundary

* Part of this work was performed at the Department of Physics, Queen Mary College, University of London.

on the number of states. Later calculations have also concentrated on the partition function since at least this is a foolproof method[1]), which avoids the intricacies of a direct calculation of the magnetic moment. A particularly careful discussion of the boundary effects on the level density for systems of large and intermediate size has been given by Dingle[5]).

A very elegant way of calculating the partition function was proposed by Sondheimer and Wilson[6]). They consider an infinite system and hence boundary effects do not enter at all. But, as pointed out by Dingle[5]), in this way one does not deal with quite the whole problem, since it is taken for granted that the susceptibility is purely a volume effect. Moreover, as will be shown below, the Sondheimer–Wilson theory suffers from an inherent contradiction. Although the partition function leads to the correct value for the magnetic moment, one finds by direct calculation that the current density and hence the magnetic moment vanishes identically.

This paper deals with a model situation for which not only the partition function, but also the local current density can be evaluated exactly. We consider an ideal electron gas confined by a cylindrically symmetric harmonic potential. The density matrix can be evaluated by the method of Sondheimer and Wilson[6]) and we find the remarkable result that in the presence of the magnetic field and with Boltzmann statistics the electron gas rotates uniformly. We also evaluate the Wigner distribution function which turns out to have an interesting form. We confine ourselves here to Boltzmann statistics.

To our knowledge the harmonic potential is the only case where such simple results can be obtained. It allows one to discuss in detail the effects of the boundary and the way in which the bulk limit is attained. For the partition function this was already done by Darwin[7]). In our view the present calculation in combination with Sondheimer and Wilson's method for treating the Fermi–Dirac case provides an attractive and lucid description of the diamagnetism of free electrons in metals. The detailed calculation of the local properties of the high temperature gas, as presented here, may also be of some interest to plasma physicists.

2. Density matrix for electrons in a harmonic potential and a magnetic field

We consider a gas of non-interacting electrons of charge $-e$, mass m, confined by a two-dimensional harmonic potential $V(r) = \frac{1}{2}K(x^2 + y^2)$ and under the influence of a uniform magnetic field B in the z-direction. We choose the cylindrical gauge for the vector potential $A(r) = (-\frac{1}{2}By, \frac{1}{2}Bx, 0)$. The single-electron hamiltonian reads

$$\mathcal{H} = \frac{1}{2m}\left(p_x - \frac{eB}{2c}y\right)^2 + \frac{1}{2m}\left(p_y + \frac{eB}{2c}x\right)^2 + \frac{p_z^2}{2m} + \tfrac{1}{2}K(x^2 + y^2). \tag{2.1}$$

Introducing the Larmor frequency ω_L and the modified frequency Ω_L by

$$\omega_L = eB/2mc, \qquad \Omega_L = (\omega_L^2 + \omega_0^2)^{\frac{1}{2}}, \qquad \omega_0^2 = K/m, \tag{2.2}$$

one can write the hamiltonian in the alternative form

$$\mathscr{H} = p^2/2m + \omega_L (xp_y - yp_x) + \tfrac{1}{2}m\Omega_L^2 (x^2 + y^2). \tag{2.3}$$

In Boltzmann statistics the single-particle density matrix satisfies the Bloch equation

$$\frac{\partial \varrho}{\partial \beta} = -\mathscr{H}\varrho. \tag{2.4}$$

In coordinate representation this becomes explicitly the partial differential equation

$$\frac{\partial \varrho(\boldsymbol{r}, \boldsymbol{r}')}{\partial \beta} = \left[\frac{\hbar^2}{2m}\nabla^2 + i\hbar\omega_L\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) - \tfrac{1}{2}m\Omega_L^2 (x^2 + y^2)\right]\varrho(\boldsymbol{r}, \boldsymbol{r}'; \beta). \tag{2.5}$$

Following Sondheimer and Wilson[6]) we look for a solution of the form

$$\begin{aligned}\varrho(\boldsymbol{r}, \boldsymbol{r}'; \beta) = f(\beta) \exp [&-ig(\beta)(x'y - y'x) + h(\beta)(xx' + yy') \\ &- \tfrac{1}{2}k(\beta)(x^2 + y^2 + x'^2 + y'^2) - (m/2\beta\hbar^2)(z - z')^2].\end{aligned} \tag{2.6}$$

This satisfies (2.5) provided the functions $f(\beta)$, $g(\beta)$, $h(\beta)$, $k(\beta)$ obey a set of coupled nonlinear ordinary differential equations which must be solved with the condition that (2.6) reduces to the well-known free particle solution for $B = 0$ and $K = 0$. One finds, putting $\mathscr{E}_L = \hbar\Omega_L$ and $\varepsilon_L = \hbar\omega_L$,

$$\begin{aligned} f(\beta) &= \left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2} \frac{\beta\mathscr{E}_L}{\sinh \beta\mathscr{E}_L}, \qquad g(\beta) = \frac{m\mathscr{E}_L}{\hbar^2}\frac{\sinh \beta\varepsilon_L}{\sinh \beta\mathscr{E}_L}, \\ h(\beta) &= \frac{m\mathscr{E}_L}{\hbar^2}\frac{\cosh \beta\varepsilon_L}{\sinh \beta\mathscr{E}_L}, \qquad k(\beta) = \frac{m\mathscr{E}_L}{\hbar^2}\coth \beta\mathscr{E}_L. \end{aligned} \tag{2.7}$$

Now one can evaluate the partition function

$$Z = \operatorname{Tr}\varrho = \int \varrho(\boldsymbol{r}, \boldsymbol{r}; \beta)\, d\boldsymbol{r}. \tag{2.8}$$

We limit the integration over z in (2.8) to the range $0 \leqslant z \leqslant C$. From (2.6) and (2.7) one finds

$$Z = Z_{xy}Z_z, \tag{2.9}$$

where

$$Z_z = C\,(m/2\pi\beta\hbar^2)^{\frac{1}{2}} \tag{2.10}$$

is the partition function corresponding to the free motion in the z-direction, and

$$Z_{xy} = \frac{\frac{1}{2}}{\cosh \beta\mathscr{E}_L - \cosh \beta\varepsilon_L} \tag{2.11}$$

is the partition function corresponding to the motion in the x and y-directions.

Hence one can evaluate the average magnetic moment and the average energy per electron. For the magnetic moment one finds

$$\langle M_z \rangle = k_B T \frac{\partial \ln Z}{\partial B} = -\mu_B \frac{\xi \sinh \beta\mathscr{E}_L - \sinh \beta\varepsilon_L}{\cosh \beta\mathscr{E}_L - \cosh \beta\varepsilon_L}, \tag{2.12}$$

where $\mu_B = e\hbar/2mc$ is the Bohr magneton, and $\xi = \omega_L/\Omega_L$. For the average energy one finds

$$\langle \mathscr{H} \rangle = -\partial \ln Z/\partial\beta = \frac{\mathscr{E}_L \sinh \beta\mathscr{E}_L - \varepsilon_L \sinh \beta\varepsilon_L}{\cosh \beta\mathscr{E}_L - \cosh \beta\varepsilon_L} + \frac{1}{2\beta}. \tag{2.13}$$

The last term is the kinetic energy in the z-direction.

3. Number density and current density

The number density per electron is given by

$$n(r) = \varrho\,(r, r)/Z \tag{3.1}$$

and from (2.6), (2.7) and (2.11) one finds the gaussian distribution

$$n(r) = \frac{\alpha}{\pi C} \exp\,[-\alpha\,(x^2 + y^2)], \tag{3.2}$$

where

$$\alpha = k - h = \frac{m\mathscr{E}_L}{\hbar^2} \frac{\cosh \beta\mathscr{E}_L - \cosh \beta\varepsilon_L}{\sinh \beta\varepsilon_L}. \tag{3.3}$$

The probability current density is given by

$$j(r) = Z^{-1} \frac{\hbar}{2mi} [\nabla\varrho\,(r, r') - \nabla'\varrho\,(r, r')]\big|_{r'=r} + \frac{e}{mc} n(r)\,A(r), \tag{3.4}$$

where as before $A(r) = (-\frac{1}{2}By, \frac{1}{2}Bx, 0)$. Substituting from (2.6) one finds that the current density can conveniently be written as the product of number density and flow velocity[8])

$$j(r) = n(r)\, V(r), \tag{3.5}$$

where the flow velocity is given explicitly by

$$V(r) = \omega_L \left(1 - \frac{\sinh \beta\varepsilon_L}{\xi \sinh \beta\mathscr{E}_L}\right)(-y, x, 0). \tag{3.6}$$

Thus we have found the remarkable result that the electron gas rotates uniformly about the z-axis.

One easily checks that the total magnetic moment

$$\langle M_z \rangle = \frac{e}{2c} \int (r \times j(r))_z \, dr, \tag{3.7}$$

as calculated from the preceding equations agrees with the result (2.12) found from the partition function. From the fact that $(\sinh x)/x$ is monotonically increasing for positive x it follows that the angular velocity in (3.6) has the same sign for any value of the field. The response of the system is diamagnetic for any field strength.

For weak field one finds from (3.3), with $\varepsilon_0 = \hbar\omega_0$,

$$\alpha \approx (m/\hbar^2)\, \varepsilon_0 \coth \beta\varepsilon_0 \quad \text{(small } B\text{)}, \tag{3.8}$$

i.e., the width of the distribution then is determined by the harmonic potential. In this limit one finds for the flow velocity

$$V(r) \approx \omega_L \left(1 - \frac{\beta\varepsilon_0}{\sinh \beta\varepsilon_0}\right)(-y, x, 0) \qquad \text{(small } B\text{)} \tag{3.9}$$

so that the magnetic moment is proportional to the field strength. From (2.12) one finds

$$\langle M_z \rangle \approx -\mu_B \beta\varepsilon_L \frac{[(\sinh \beta\varepsilon_0)/\beta\varepsilon_0] - 1}{\cosh \beta\varepsilon_0 - 1} \qquad \text{(small } B\text{)}. \tag{3.10}$$

For strong field one finds from (3.3)

$$\alpha \approx \tfrac{1}{2}\beta m\omega_0^2 \qquad \text{(large } B\text{)} \tag{3.11}$$

i.e., the width of the distribution is again determined by the harmonic potential but it now has a value as if the system were classical. The flow velocity tends

monotonically to a finite value

$$V(\boldsymbol{r}) \approx \tfrac{1}{2}\beta\hbar\omega_0^2\,(-y, x, 0) \qquad \text{(large } B\text{)}. \tag{3.12}$$

Hence the magnetic moment saturates, and from (2.12) or (3.7) one finds for the limiting value

$$\langle M_z \rangle \approx -\mu_B \qquad \text{(large } B\text{)}. \tag{3.13}$$

From (2.13) the average energy becomes for strong field

$$\langle \mathscr{H} \rangle \approx \varepsilon_L \quad \text{(large } B\text{)}. \tag{3.14}$$

Thus in the strong field limit one arrives at the following simple picture: The electrons orbit in the ground state of the cyclotron motion and constitute magnetic dipoles of strength equal to the Bohr magneton. These dipoles are distributed in space in a classical distribution which rotates uniformly. Since the kinetic energy becomes large the uncertainty principle allows precise classical localization in the directions normal to the field.

4. Limit of weak potential

The parameter $K^{-\frac{1}{2}}$ can be regarded as characterizing the dimensions of the system transverse to the field. The results of the preceding section apply to systems of any size. In order to make the connection with the Landau theory[4]) of diamagnetism for macroscopic bodies it is necessary to consider the limit of weak potential, thus allowing the dimensions normal to the field to grow indefinitely. From (3.3) one finds that in this limit the width of the spatial distribution is determined by

$$\alpha \approx \tfrac{1}{2}\beta m\omega_0^2 \qquad \text{(small } K\text{)}, \tag{4.1}$$

which is again the classical value. The flow velocity becomes

$$V(\boldsymbol{r}) \approx \frac{1}{2}\,\frac{\omega_0^2}{\omega_L}\,(\beta\varepsilon_L \coth \beta\varepsilon_L - 1)\,(-y, x, 0) \qquad \text{(small } K\text{)} \tag{4.2}$$

and the magnetic moment

$$\langle M_z \rangle \approx -\mu_B \left(\coth \beta\varepsilon_L - \frac{1}{\beta\varepsilon_L}\right) \qquad \text{(small } K\text{)}. \tag{4.3}$$

Thus in this limit the magnetic moment tends to a value independent of the potential. The function in brackets in (4.3) is just the Langevin function. The same value for the moment is obtained from the partition function as calculated in the absence of any potential[6]).

It is to be noted that the flow velocity $V(r)$ in (4.2) tends to zero with K. On the other hand the width of the distribution increases indefinitely as K tends to zero. The two effects just compensate each other and lead in the limit to a finite value for the magnetic moment, given by (4.3). Correct understanding of the physical situation requires carrying out the above limiting procedure. If one considers free particles from the start, as done by Sondheimer and Wilson[6]), one finds the contradictory result that the current density vanishes, whereas at the same time the partition function leads to a finite value for the magnetic moment.

If one takes the limit of small B in (4.3) one finds

$$\langle M_z \rangle \approx -\tfrac{1}{3}\mu_B \beta \varepsilon_L \quad \text{(small } K\text{, small } B\text{)}. \tag{4.4}$$

This value is also found by taking the limit of small K in eq. (3.10). Hence the two limits can be interchanged. For large B the magnetic moment again saturates to the value $\langle M_z \rangle \approx -\mu_B$, in agreement with (3.13).

5. Wigner distribution function

The classical results are recovered by taking the limit $\hbar \to 0$. Thus one finds

$$\begin{aligned} &\langle M_z \rangle = 0, \qquad \langle \mathcal{H} \rangle = 5/2\beta, \\ &\alpha = \tfrac{1}{2}\beta m\omega_0^2, \qquad V = 0. \end{aligned} \qquad (\hbar \to 0) \tag{5.1}$$

The magnetic moment vanishes in agreement with Miss van Leeuwen's theorem[2]). The theorem also implies that locally the current density vanishes.

The relation between the classical and quantum-mechanical results is seen more clearly by rephrasing the latter in terms of the Wigner distribution function[9]). We introduce central and relative coordinates by

$$\boldsymbol{R} = \tfrac{1}{2}(\boldsymbol{r} + \boldsymbol{r}'), \qquad \boldsymbol{q} = \boldsymbol{r}' - \boldsymbol{r}. \tag{5.2}$$

The Wigner distribution function $f_W(\boldsymbol{R}, \boldsymbol{P}; \beta)$ is defined by

$$f_W(\boldsymbol{R}, \boldsymbol{P}; \beta) = h^{-3} \int \varrho(\boldsymbol{R} - \tfrac{1}{2}\boldsymbol{q}, \boldsymbol{R} + \tfrac{1}{2}\boldsymbol{q}; \beta)\, e^{i\boldsymbol{P}\cdot\boldsymbol{q}/\hbar}\, d\boldsymbol{q}. \tag{5.3}$$

It is normalized to

$$\int f_W(\boldsymbol{R}, \boldsymbol{P})\, d\boldsymbol{R}\, d\boldsymbol{P} = Z. \tag{5.4}$$

Quantum-statistical averages can be evaluated from the Wigner distribution according to the rule

$$\langle F \rangle = Z^{-1} \operatorname{Tr} \varrho F = Z^{-1} \int f_{\mathrm{W}}(\boldsymbol{R}, \boldsymbol{P}) F_{\mathrm{W}}(\boldsymbol{R}, \boldsymbol{P}) \, \mathrm{d}\boldsymbol{R} \, \mathrm{d}\boldsymbol{P}, \tag{5.5}$$

where $F_{\mathrm{W}}(\boldsymbol{R}, \boldsymbol{P})$ is the Wigner equivalent of the quantum-mechanical operator F. If F is given in coordinate representation as $F(\boldsymbol{r}, \boldsymbol{r}')$ its Wigner equivalent is given by

$$F_{\mathrm{W}}(\boldsymbol{R}, \boldsymbol{P}) = \int F(\boldsymbol{R} - \tfrac{1}{2}\boldsymbol{q}, \boldsymbol{R} + \tfrac{1}{2}\boldsymbol{q}) \, \mathrm{e}^{\mathrm{i}\boldsymbol{P}\cdot\boldsymbol{q}/\hbar} \, \mathrm{d}\boldsymbol{q}. \tag{5.6}$$

For the operators of present interest the Wigner equivalents are simply related to the corresponding classical phase space functions by Weyl's rule[10]).

For the density matrix given by (2.6) the Wigner distribution can be evaluated explicitly. Before giving the result we introduce some new notation. We split the flow velocity $V(\boldsymbol{r})$ given by eq. (3.6) into a purely diamagnetic part V_{d} and a paramagnetic part V_{p},

$$V = V_{\mathrm{d}} + V_{\mathrm{p}}, \tag{5.7}$$

where

$$V_{\mathrm{d}} = \frac{e}{mc} A(\boldsymbol{r}), \qquad V_{\mathrm{p}} = -\frac{e}{mc} \frac{\sinh \beta\varepsilon_{\mathrm{L}}}{\xi \sinh \beta\mathscr{E}_{\mathrm{L}}} A(\boldsymbol{r}). \tag{5.8}$$

We also define a quantum temperature T' by $\beta' = 1/k_{\mathrm{B}}T'$ with

$$\beta' = \frac{2 \sinh \beta\mathscr{E}_{\mathrm{L}}}{\mathscr{E}_{\mathrm{L}} (\cosh \beta\mathscr{E}_{\mathrm{L}} + \cosh \beta\varepsilon_{\mathrm{L}})}. \tag{5.9}$$

The Wigner distribution can then be written in the form

$$f_{\mathrm{W}}(\boldsymbol{R}, \boldsymbol{P}; \beta) = Z \frac{\alpha}{\pi C} \frac{\beta' \beta^{\ddagger}}{(2\pi m)^{3/2}} \exp\left\{ -\frac{\beta'}{2m} [(P_x - mV_{\mathrm{p}x})^2 + (P_y - mV_{\mathrm{p}y})^2] \right.$$
$$\left. - \frac{\beta}{2m} P_z^2 - \alpha (X^2 + Y^2) \right\}. \tag{5.10}$$

Note that in the present case the distribution is everywhere positive and has a simple classical interpretation. Integrating $f_{\mathrm{W}}(\boldsymbol{R}, \boldsymbol{P})$ over the momenta $\boldsymbol{P}$ one recovers the density distribution (3.2). Integrating over the spatial coordinates one finds that the momentum distribution is given by the shifted maxwellian

$$f(\boldsymbol{P}) = \frac{\beta' \beta^{\ddagger}}{(2\pi m)^{3/2}} \exp\left\{ -\frac{\beta'}{2m} [(P_x - mV_{\mathrm{p}x})^2 + (P_y - mV_{\mathrm{p}y})^2] - \frac{\beta}{2m} P_z^2 \right\}. \tag{5.11}$$

In the classical limit β' reduces to β, and V_p becomes equal to $-V_d$. Also, α in (5.10) reduces to $\frac{1}{2}\beta m\omega_0^2$. The current density is given by

$$j(R) = \frac{1}{mZ}\int\left[P + \frac{e}{c}A(R)\right] f_W(R, P)\,dP = [V_p(R) + V_d(R)]\,n(R). \quad (5.12)$$

It is of interest to note that the parameters β' and α differ. For a simple one-dimensional harmonic oscillator with frequency ω_0 the Wigner distribution would be

$$f_W(X, P) = \left[2\pi\hbar\cosh\frac{\beta\hbar\omega_0}{2}\right]^{-1}\exp\left[-\beta''\left(\frac{P^2}{2m} + \tfrac{1}{2}m\omega_0^2X^2\right)\right] \quad (5.13)$$

with $\beta'' = (k_BT'')^{-1}$ and quantum temperature T'' given by

$$k_BT'' = \tfrac{1}{2}\hbar\omega_0\coth\tfrac{1}{2}\beta\hbar\omega_0. \quad (5.14)$$

Hence in that case kinetic and potential energy appear with the same quantum parameter. In the present situation the magnetic field not only causes the current to flow, but also affects the average transverse kinetic and potential energy.

The local transverse kinetic energy density is given by

$$\frac{1}{Z}\int\frac{1}{2m}\left[\left(P_x + \frac{e}{c}A_x\right)^2 + \left(P_y + \frac{e}{c}A_y\right)^2\right] f_W(R, P)\,dP$$
$$= [k_BT' + \tfrac{1}{2}mV^2]\,n(R) \quad (5.15)$$

and hence is the sum of a temperature and a streaming contribution. As we have seen, in the limit of weak potential, $K \to 0$, the local flow velocity V tends to zero. In this limit one finds from (5.9) for the quantum temperature

$$k_BT' \sim \varepsilon_L\coth\beta\varepsilon_L \qquad \text{(small } K\text{)} \quad (5.16)$$

which is to be compared with (5.14). Thus the cyclotron motion gives rise to a typical harmonic oscillator quantum temperature. In the limit of strong field k_BT' tends to ε_L, corresponding to the zero point cyclotron motion. As is evident from (3.3) and (5.9), for general values of B and K the parameters α and β' are influenced by both the magnetic field and the oscillator potential.

6. Particle motion

The preceding results have been obtained without inquiry into the details of the particle dynamics. A study of the particle motions reveals that the simple uniform rotation of the electron gas is a result of quite delicate additions and cancellations

of the individual motions in the Boltzmann statistics. The dynamics of the particles is most easily studied by transforming the hamiltonian (2.1) to normal modes. The transverse part of the hamiltonian is diagonalized by introduction of the following normal mode coordinates

$$a_\pm = \frac{1}{2}\left(\frac{m\Omega_L}{\hbar}\right)^{\frac{1}{2}}(x \mp iy) + \frac{i}{2(\hbar m\Omega_L)^{\frac{1}{2}}}(p_x \mp ip_y), \tag{6.1}$$

where $\Omega_L = (\omega_L^2 + \omega_0^2)^{\frac{1}{2}}$. Hence one has

$$x + iy = \left(\frac{\hbar}{m\Omega_L}\right)^{\frac{1}{2}}(a_+^\dagger + a_-), \qquad p_x + ip_y = i(\hbar m\Omega_L)^{\frac{1}{2}}(a_+^\dagger - a_-). \tag{6.2}$$

Solving for x, y, p_x, p_y and substituting in (2.1) one finds

$$\mathcal{H} = \hbar\omega_+(a_+^\dagger a_+ + \tfrac{1}{2}) + \hbar\omega_-(a_-^\dagger a_- + \tfrac{1}{2}) + p_z^2/2m, \tag{6.3}$$

where

$$\omega_\pm = \Omega_L \pm \omega_L. \tag{6.4}$$

The corresponding classical hamiltonian is obtained by putting $\hbar = 1$ in (6.1)–(6.3) and omitting the terms with $\frac{1}{2}$ in (6.3). We only discuss the case of weak potential $\omega_0 \ll \omega_L$. Then classically the electron partakes in two circular motions, a fast cyclotron motion with frequency ω_+, and a slow motion in the opposite direction with frequency ω_-. Both $a_+^\dagger a_+$ and $a_-^\dagger a_-$ are of course constants of the motion, but of particular interest is the linear combination

$$L_z = a_+^\dagger a_+ - a_-^\dagger a_- = xp_y - yp_x \tag{6.5}$$

which is the z-component of angular momentum.

Previous results for average energy and magnetic moment are recovered easily by expressing the variables in terms of the normal mode coordinates and using

$$\langle a_\pm^\dagger a_\pm\rangle = [\exp(\hbar\omega_\pm) - 1]^{-1}. \tag{6.6}$$

The magnetic moment is related to angular momentum by

$$M_z = \frac{e}{2mc}L_z + \frac{e}{2c}\omega_L(x^2 + y^2). \tag{6.7}$$

From (6.5) and (6.6) it follows that $\langle L_z\rangle$ is always negative. In the classical case $\langle L_z\rangle$ just balances the average of the second term in (6.7) to give zero magnetic moment.

The results for the local number density and current density are obtained more easily by the method of sections 2 and 3.

From (6.3) it follows that the energy eigenvalues are given by

$$E(n_+, n_-, k_z) = \hbar\omega_+ (n_+ + \tfrac{1}{2}) + \hbar\omega_- (n_- + \tfrac{1}{2}) + \hbar^2 k_z^2/2m, \tag{6.8}$$

and one easily writes down the corresponding eigenfunctions in terms of normal mode coordinates. On the other hand one can also solve the Schrödinger equation directly in coordinate representation. The eigenfunctions are in cylindrical coordinates

$$\psi(r) = \phi_{n,l}(r, \varphi)\, e^{ik_z z} \tag{6.9}$$

with

$$\phi_{nl}(r, \varphi) = \pi^{-\frac{1}{2}} \left(\frac{n!\, b^{|l|+1}}{\Gamma(n + |l| + 1)} \right)^{\frac{1}{2}} r^{|l|} L_n^{|l|}(br^2)\, e^{-\frac{1}{2}br^2 + il\varphi}, \tag{6.10}$$

where $b = m\Omega_L/\hbar^2$, and $L_n^{|l|}$ are the associated Laguerre polynomials. The quantum number n runs over 0, 1, 2, ..., and l over the positive and negative integers. The functions $\phi_{n,l}(r, \varphi)$ form an orthonormal set. The corresponding energy eigenvalues are

$$E(n, l, k_z) = (2n + |l| + 1)\hbar\Omega_L + l\hbar\omega_L + \hbar^2 k_z^2/2m. \tag{6.11}$$

From (6.5) and (6.8) it follows that

$$l = n_+ - n_-, \qquad n = \tfrac{1}{2}(n_+ + n_-) - \tfrac{1}{2}|n_+ - n_-|. \tag{6.12}$$

The results of sec. 2 for the density matrix can be recovered by using the identities[11])

$$\sum_{n=0}^{\infty} \frac{n!}{\Gamma(n + |l| + 1)} L_n^{|l|}(\xi) L_n^{|l|}(\eta) \zeta^n = \frac{(\xi\eta\zeta)^{-\frac{1}{2}|l|}}{1 - \zeta} I_l\left(\frac{2(\xi\eta\zeta)^{\frac{1}{2}}}{1 - \zeta} \right) \exp\left(-\frac{\zeta}{1 - \zeta}(\xi + \eta) \right), \tag{6.13}$$

$$\sum_{l=-\infty}^{\infty} t^l I_l(u) = \exp[\tfrac{1}{2}u(t + t^{-1})],$$

where $I_l(u)$ are the Bessel functions of imaginary argument. This demonstrates again the delicate balance of the individual eigenmodes giving rise to the simple macroscopic behavior described above.

References

1) See review by Van Vleck, J.H., Nuovo Cim. Supp. **6** (1957) 857.
2) J.H. van Leeuwen, Dissertation, Leiden (1919); J. de Phys. **2** (1921) 361.
See also J.H. van Vleck, The Theory of Electric and Magnetic Susceptibilities (Oxford Univ. Press, London, 1932) p. 94.
3) N. Bohr, Dissertation, Copenhagen (1911).
4) L. Landau, Z. Phys. **64** (1930) 629.
5) R.B. Dingle, Proc. Roy. Soc. **A211** (1952) 500, 517.
6) E.H. Sondheimer and A.H. Wilson, Proc. Roy. Soc. **A210** (1951) 173.
See also A.H. Wilson, Theory of Metals (Cambridge Univ. Press, Cambridge, 1953) p. 160.
7) C.G. Darwin, Proc. Camb. Phil. Soc. **27** (1930) 86.
8) B.U. Felderhof, Physica **71** (1974) 41.
9) E. Wigner, Phys. Rev. **40** (1932) 749.
10) K. Schram and B.R.A. Nijboer, Physica **25** (1959) 733.
11) I.S. Gradshteyn and I.M. Ryzhik, Table of Integrals, Series and Products (Academic Press, New York, 1965) 8.511.1 and 8.976.1.