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THE RAYLEIGH MODEL: SINGULAR TRANSPORT THEORY IN ONE DIMENSION

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CONTENTS

We present a comprehensive account of the special 'Rayleigh piston' model for the spatial and velocity relaxation of an ensemble of labelled test-particles in a one-dimensional heat-bath of particles with identical mass. This model, originally formulated by Rayleigh in 1891 but since largely neglected, is in effect a prototype for all later models in singular particle transport theory and serves to illustrate the mathematical problems associated with the occurrence of singular eigenfunctions and continuous spectra of a scattering operator. Although other idealized scattering models are known, the Rayleigh model remains a unique example of an exactly soluble singular system which, in including conservation laws and time-reversal symmetry in scattering, retains a degree of mechanical realism.

1. Introduction

In the study of model relaxation equations that approximate the behaviour of real gas-kinetic systems two major sources of difficulty attend even the most elementary treatments. On the one hand we have the essential nonlinearity of the collision terms governing the evolution of the closed system through the Boltzmann equation, on the other there is the *singular* nature of the corresponding operators which enters unavoidably even in linearized treatments of relaxation and particle transport. Both these aspects have received considerable attention in recent years, the former largely in the context of rare gas dynamics, the latter primarily in relation to the equations of neutron transport. In both linear and nonlinear treatments the discovery of soluble models has played an important part; while these are undoubtedly hard to find, those that have emerged are of all the more value and in some cases have revealed unsuspected generalizations. The Bobylev–Krook–Wu model Boltzmann equation is a notable example in this respect (Bobylev 1976, Krook & Wu 1977).

Like Boltzmann models, linear transport models are most tractable when reduced either to scalar form in three dimensions or to 'vector' (i.e. full-range) form in one. While the latter is in an obvious sense unrealistic, there are grounds for the belief that at least some of the mathematical essence of the real system remains in one dimension, whatever geometrical features may be falsified. This is certainly true of the *singular* nature of the eigenvalue problems arising which lead, by one route or another, to the problematics of distribution theory and continuous spectra. It is with this aspect that we shall be mainly concerned in this paper; a parallel treatment of model nonlinear equations will be found elsewhere (Futcher & Hoare 1982).

There are two quite distinct models for the statistical dynamics of the one-dimensional gas. The first, studied extensively by Jepsen (1965), Lebovitz *et al.* (1968) and Levitt (1973) is concerned with the motion of a string of non-penetrating particles constrained on a line in the manner of an abacus. When the particles have equal mass, the property that neighbouring elements simply exchange velocities on collision leads to an exact solution for the position–velocity correlation function for a single particle, but by the same token cannot lead to any net velocity relaxation overall. This and the somewhat unnatural 'rattling' correlations which are found limit the value of the Jepsen model as a prototype for three-dimensional behaviour.

An alternative is to consider a notional heat-bath with which an ensemble of labelled test-particles interact, the heat-bath particles always presenting an aspect of 'molecular chaos' and being 'spirited away' after each collision. This is, in effect, the Rayleigh model, first formulated in 1891 and investigated more recently by a number of authors (Rayleigh 1891, Green 1951, Van Kampen 1955, 1961, Akama & Siegel 1965, Hoare & Rahman 1973, 1974, 1976, Barker *et al.* 1977 and Résibois 1978). Though it lacks the element of true N-body mechanics present in the Jepsen model, it does exhibit velocity relaxation and equilibrium fluctuations and a well defined approach to Brownian motion in the limit of very heavy test-particles. Moreover it is the correct one-dimensional analogue of the equation of particle transport in a moderator, for which a large, independent literature exists (see for example Williams 1966, 1971, Hoare 1971).

Although both models lead to subtle solutions, those of the Rayleigh model might be said to be the more interesting inasmuch as they can be expressed through the eigenfunctions of a singular integral operator and may in turn act as a set of 'basis-distributions' for the expansion of other one-dimensional initial-value problems with 'non-L_2' character. We have already shown how the Rayleigh scattering operator for equal system and heat-bath masses, and Maxwellian bath-distribution, leads to eigenfunctions of Hadamard-pseudofunction type with quadratic singularity and an infinite continuous spectrum above a threshold (Hoare & Rahman 1974); here we shall complete the analysis of the 'special Rayleigh problem' in these terms, extending our results to non-Maxwellian heat-baths and to the spatially inhomogeneous case.

As we earlier indicated, our interest in the Rayleigh problem is in large part methodological. Nowhere, so far as we know, has an exact solution been given for a singular master equation that, however simplified, remains 'dynamically realistic'. By this we mean that the simplification is only geometrical, conservation laws and time-reversal symmetry being correctly reproduced. Of the very few singular models available so far (e.g. the 'one-velocity' model of Case (1959, 1960) (see especially Case & Zweifel 1967)) none seems to preserve this minimum of physical consistency.

It is widely acknowledged that a certain paradoxical character attaches to singular transport theory. While, formally at least, solutions may be given in terms of the eigenfunctions of the appropriate integral operators, the derivations involved are problematic, particularly in dimensions higher than one, and the completeness of the solution set is not as a rule easy to establish. Notwithstanding this, it is somewhat unreadily admitted that, even in otherwise intractable cases, a naïve application of a Laplace or Mellin transform can sometimes lead to straightforwardly computable solutions that require only 'elementary' methods. While distribution theory and transform methods are well known to be closely interconnected, the lack of soluble models has so far prevented a detailed comparison of the two for any physically realistic singular operator.

In the present work, which we hope to make a definitive account of the 'special Rayleigh problem', we shall show that it is possible to compare singular eigenfunction and transform solutions in such a way that each illuminates the other, while at the same time leading to computationally useful algorithms. Indeed we shall be able to show that a proper formulation of the model practically forces us to adopt the Bremmerman–Durand approach to distribution theory (Bremmerman & Durand 1961, Bremmerman 1965) according to which distributions are represented by the discontinuities of certain analytic functions across the real axis. In these terms the representation of singular eigendistributions has not only the virtues of simplicity but also circumvents technical problems, particularly in the demonstration of completeness.

This paper falls into four parts. After an initial analysis of the spatially homogeneous model (§ 2) we describe the singular eigenfunctions for the same in some detail, establishing the orthogonality and completeness of the two parity types by 'distributional' methods and giving a proper account of the Fourier expansion of the initial-value solution for the particle velocity distribution in the singular basis (§ 3). This extends and completes the previous account of Hoare & Rahman (1974) while correcting certain misconceptions in it. We then consider the Laplace transform solution to the same problem and arrive at the time-dependent velocity distribution for the ensemble by this route (§ 4). By reduction of the inverse transformation to real integrals we then obtain the Bremmerman formulation of the original singular eigenfunctions. From this unified standpoint other properties of the system, in particular the velocity autocorrelation function and the linear-response approximation to the complex admittance for charged test-particles, are derived (§ 5). In § 6 we go on to consider the passage-time statistics for transport to either an upper or a lower absorbing barrier. The former would appear to be a, so far, unique example of an exactly soluble barrier problem with singular transition operator. Finally we turn to the spatially inhomogeneous problem (§ 7). Here it is also possible to find an exact solution to the position–velocity distribution function, at least to within a Fourier–Laplace transform. Taking appropriate initial conditions we are then able to derive corresponding expressions for the Van Hove space–time correlation function and its transforms, which may be used to test certain statistical approximations, such as the 'Gaussian' approximation of Vineyard.

2. The general relaxation problem

2.1. *The transport equation*

Our primary concern in this paper will be with solutions to the integro-differential equation

$$\left(\frac{\partial}{\partial \tau}+v\frac{\partial}{\partial x}\right)p(x,v,\tau) = \int_{-\infty}^{\infty} \mathrm{d}u\,[k(v,u)\,p(x,u,\tau)-k(u,v)\,p(x,v,\tau)], \tag{2.1}$$

and its simplifications. In this p represents the time-dependent spatial and velocity distribution function for an ensemble of test-particles interacting with a heat bath of particles within general $v \in (-\infty, +\infty)$, $x \in (-\infty, +\infty)$. The *transition kernel* $k(u, v)$ is the rate constant for transitions $u \to \mathrm{d}v$ about v in velocity state-space per unit time. We take the independent variables x, v, τ to be dimensionless reductions of the true variables X, V, t, obtained by a procedure to be given, and the dependent ones p and k to conform to these under the normalizations

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{d}v\,p(x, v, \tau) = 1, \tag{2.2}$$

and

$$\int_{-\infty}^{\infty} \mathrm{d}u\,k(v, u) = z(v), \tag{2.3}$$

where $z(v)$ is the collision number per unit time for a particle of reduced velocity v. An alternative to equation (2.1) is thus

$$\left[\frac{\partial}{\partial \tau} + v\frac{\partial}{\partial x} + z(v)\right] p(x, v, \tau) = \int_{-\infty}^{\infty} \mathrm{d}u\,k(v, u)\,p(x, u, \tau). \tag{2.4}$$

Here the 'gain' and 'loss' terms due to collisions and free streaming are easily identifiable. For a spatially homogeneous test-particle ensemble the above simplifies to

$$\left[\frac{\partial}{\partial \tau} + z(v)\right] p(v, \tau) = \int_{-\infty}^{\infty} \mathrm{d}u\,k(v, u)\,p(u, \tau), \tag{2.5}$$

which may be written symbolically as

$$(\partial/\partial\tau)\,p = -\mathscr{A}p, \tag{2.6}$$

with $\mathscr{A}$ an integral operator with kernel A:

$$A(u, v) = -k(u, v) + z(v)\,\delta(u-v). \tag{2.7}$$

The occurrence of the *multiplicative operator* $z(v)$ here indicates the singular nature of the problem. Equations (2.1) and (2.5) represent simple relaxation behaviour without sources or sinks and we shall thus be considering solutions to the initial-value problems in which $p(x, v, 0)$ or $p(v, 0)$ are specified at zero time together with the kernel $k(u, v)$.

2.2. *The special Rayleigh model*

The general Rayleigh model, in which a test-particle of mass M responds to a one-dimensional heat-bath of particles of mass m leads to a somewhat complicated form for $k(u, v)$ which, though now qualitatively well understood (Hoare & Rahman 1973, Barker *et al.* 1981) has so far resisted all attempts at an analytic solution. In the *special* Rayleigh model, to which we confine our attention here, labelled test-particles are dilutely dispersed in a heat-bath of atoms of identical mass $(M = m)$, the latter having a given distribution $H_0(V)$ in the (true) velocity variable (figure 1). Since under these conditions the colliding particles merely exchange velocities, the corresponding transition kernel takes on the particularly simple form

$$K(U, V) = C|U-V|H_0(V), \tag{2.8}$$

with C a constant including the number density and cross section of the particles concerned. Still in unscaled variables we can write the collision number function

$$Z(V) = C\int_{-\infty}^{\infty} \mathrm{d}U|V-U|H_0(U). \tag{2.9}$$

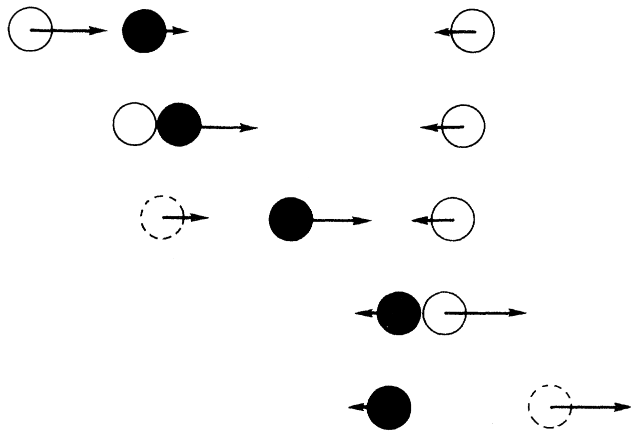

FIGURE 1. A collision sequence of the special Rayleigh model. The test-particle (black) undergoes random collisions with heat-bath particles (white) of equal mass, such that velocities are exchanged on impact. The heat-bath particles 'materialize' at random and 'vanish' after each impact. Two successive collisions are illustrated, the first of 'knocking-on' type the second of 'head-on' type. In the sequence shown the time-intervals implied are approximately equal.

We shall assume, without serious loss of generality, that the velocity distribution of the heat-bath is isotropic, namely that $H_0(-V) = H_0(V)$, such that $Z(-V) = Z(V) = 2Z(|V|)$ (half-range normalization being assumed for $Z(|V|)$). As Rayleigh himself pointed out, it is not necessary for further progress to assume that $H_0(V)$ is in fact a Maxwellian.

The value of $Z(0)$, the collision number for *stationary* test-particles is of particular importance since evidently

$$Z(0) = 2C\int_0^\infty \mathrm{d}U\, UH_0(U) = CV_0 = t_0^{-1}, \tag{2.10}$$

with V_0 the appropriate mean speed. The characteristic time t_0 and velocity V_0 can now be used to scale time and velocity as well as the distance variable (X). In this way we are led to the reductions

$$\begin{aligned} u &= U/V_0, \quad h_0(v) = V_0 H_0(vV_0),\\ v &= V/V_0, \quad p(x,v,\tau) = V_0^2 Z(0)^{-1} P(xV_0/Z(0), vV_0, \tau/Z(0)),\\ \tau &= Z(0)\,t, \quad k(u,v) = Z(0)^{-1} K(uV_0, vV_0),\\ x &= (Z(0)/V_0)\,X, \quad z(v) = Z(vV_0). \end{aligned}$$

For the Rayleigh model, the spatially homogeneous transport equation thus reads

$$\frac{\partial p(v,\tau)}{\partial \tau} = h_0(v)\int_{-\infty}^{\infty} \mathrm{d}u\,|v-u|\,p(u,\tau) - z(v)\,p(v,\tau). \tag{2.11}$$

It is with this equation that we shall be concerned throughout the next sections. We shall begin by considering the most important properties of the transition kernel $k(u,v) = h_0(v)|v-u|$ and its collision-number function $z(v)$.

2.3. *Properties of the transition kernel*

Most fundamentally the transition kernel $k(u,v)$ shows three symmetry properties:

(*a*) *detailed balance* for reversed collisions,

$$h_0(v)\,k(v,u) = h_0(u)\,k(u,v); \tag{2.12}$$

(*b*) *inverse collisional symmetry*, $\quad k(u,-v) = k(-u,v);$ (2.13)

(*c*) *parity decomposition*, $\quad k(u,v) = k_{ev}(u,v) + k_{od}(u,v),$

where

$$k_{ev}(u,v) = h_0(u)\max(|u|,|v|) \tag{2.14}$$

and

$$k_{od}(u,v) = -h_0(u)\,\mathrm{sgn}\,(u)\,\mathrm{sgn}\,(v)\min(|u|,|v|). \tag{2.15}$$

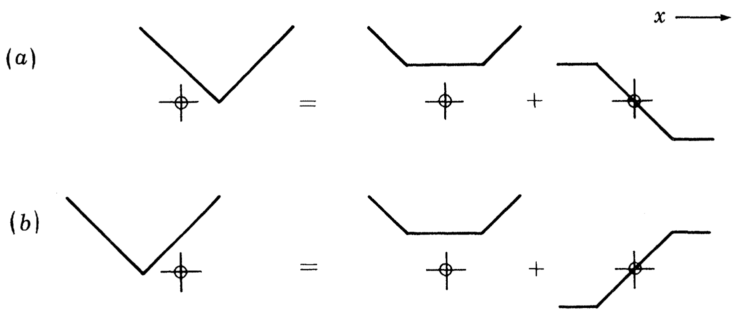

FIGURE 2. Graphical demonstration of the parity decomposition of the function $f(x,y) = |x-y|$. Left, the function $|x-y|$ for given $y > 0$, (*a*), and $y < 0$, (*b*). Right, the even component $\max(|x|, |y|)$ and odd component $-\mathrm{sgn}\,(x)\,\mathrm{sgn}\,(y)\min(|x|,|y|)$ for the two cases.

The last two equations arise from the little known and amusing identity

$$|x-y| = \underset{\text{(even)}}{\max(|x|,|y|)} - \underset{\text{(odd)}}{\mathrm{sgn}\,(x)\,\mathrm{sgn}\,(y)\min(|x|,|y|)}, \tag{2.16}$$

which is illustrated in figure 2. (See also Appendix 1.)

It follows immediately from (2.12) that the function $h_0(x)$ satisfies the transport equation with the left-hand side zero. Thus $p(v,\infty)$ $(=h_0(v))$ is stationary under the action of $k(u,v)$:

$$\int_{-\infty}^{\infty} \mathrm{d}u\,k(u,v)\,h_0(u) = z(v)\,h_0(v). \tag{2.17}$$

At the same time we note that it is possible to define an operator and symmetric kernel

$$\mathscr{G} \equiv G(u,v) = k(u,v)\,[h_0(u)/h_0(v)]^{\frac{1}{2}} = G(v,u), \tag{2.18}$$

in terms of which the transport equation (2.5) may be reduced to symmetric (self-adjoint) form. Thus, by defining the new dependent variable $\rho(v,\tau) = h_0(v)^{-\frac{1}{2}}p(v,\tau)$ we have that

$$\left[\frac{\partial}{\partial\tau} + z(v)\right]p(v,\tau) = \int_{-\infty}^{\infty} \mathrm{d}u\,[h_0(v)\,h_0(u)]^{\frac{1}{2}}\,|u-v|\,p(u,\tau). \tag{2.19}$$

The effect of the parity decomposition (*c*) above on the physical interpretation of the model is of considerable importance. On defining the parity components

$$p_{ev}(v,\tau) = \tfrac{1}{2}[p(v,\tau) + p(-v,\tau)] \tag{2.20}$$

and

$$p_{od}(v,\tau) = \tfrac{1}{2}[p(v,\tau) - p(-v,\tau)], \tag{2.21}$$

it follows that the equation $(\partial p/\partial \tau) = -\mathscr{A}p$ can be decomposed into the separate relations

$$\partial p_{\mathrm{ev}}/\partial \tau = -\mathscr{A}_{\mathrm{ev}} p_{\mathrm{ev}}, \tag{2.22}$$

$$\partial p_{\mathrm{od}}/\partial \tau = -\mathscr{A}_{\mathrm{od}} p_{\mathrm{od}}, \tag{2.23}$$

with operators corresponding to the kernels

$$\mathscr{A}_{\mathrm{ev}} \equiv A_{\mathrm{ev}}(u,v) = -2\max(|u|,|v|)\,h_0(v) + z(u)\,\delta_{\mathrm{ev}}(u,v), \tag{2.24}$$

$$\mathscr{A}_{\mathrm{od}} \equiv A_{\mathrm{od}}(u,v) = \operatorname{sgn}(u)\operatorname{sgn}(v)\min(|u|,|v|)\,h_0(v) + z(u)\,\delta_{\mathrm{od}}(u,v). \tag{2.25}$$

Here $\delta_{\mathrm{ev}}(u,v)$ and $\delta_{\mathrm{od}}(u,v)$ are parity components of the δ-function defined (see Appendix 1) as

$$\delta_{\mathrm{ev}}(x,y) = \tfrac{1}{2}[\delta(x-y)+\delta(x+y)], \tag{2.26}$$

$$\delta_{\mathrm{od}}(x,y) = \tfrac{1}{2}[\delta(x-y)-\delta(x+y)]. \tag{2.27}$$

However, on constructing equations (2.22) and (2.23) explicitly, we find further simplifications to

$$\frac{\partial p_{\mathrm{ev}}(v,\tau)}{\partial \tau} = 2h_0(v)\int_0^\infty \mathrm{d}u\, p_{\mathrm{ev}}(u,\tau)\max(|v|,u) - z(v)\,p_{\mathrm{ev}}(v,\tau), \tag{2.28}$$

and
$$\frac{\partial p_{\mathrm{od}}(v,\tau)}{\partial \tau} = -2\operatorname{sgn}(v)\,h_0(v)\int_0^\infty \mathrm{d}u\min(|v|,u)\,p_{\mathrm{od}}(u,\tau) - z(v)\,p_{\mathrm{od}}(v,\tau). \tag{2.29}$$

The physical content of these equations is that the first governs the particle *speed* distribution $p(|v|,\tau)$, the second the *flux* of test particles $F(v,\tau) = |v|\,p_{\mathrm{od}}(v,\tau)$. Making the natural association $p_{\mathrm{ev}}(v,\tau) = \tfrac{1}{2}p(|v|,\tau)$, the latter now being *half-range* normalized, we obtain

$$\int_0^\infty \mathrm{d}v\, p(|v|,\tau) = 1, \tag{2.30}$$

and noting similarly that $z(|v|) = 2z(v)$, $h_0(|v|) = 2h_0(v)$, $v \in (0,\infty)$, we find for the speed transport equation

$$\partial p(|v|,\tau)\,\partial\tau = -\mathscr{B}p(|v|,\tau), \tag{2.31}$$

with $\mathscr{B}$ the half-range operator

$$\mathscr{B} \equiv B(u,v) = h_0(|v|)\max(|u|,|v|) - z(v)\,\delta(|u|-|v|). \tag{2.32}$$

As here, we shall keep modulus signs whenever ambiguity is possible, but omit them otherwise.

It is the flux $F(v,\tau)$ rather than $p(v,\tau)$ that is the usual quantity of interest in neutron transport calculations. In one dimension the positive and negative signs for F indicate motion to the right and left respectively, while the total flux,

$$F_{\mathrm{tot}}(\tau) = \int_{-\infty}^\infty \mathrm{d}v\, v\, p(v,\tau) = \langle v(\tau)\rangle, \tag{2.33}$$

is clearly identical with the mean particle velocity at time τ. Thus as $p_{\mathrm{ev}}(v,\tau)$ and $p(|x|,\tau)$ tend to the equilibrium values $h_0(v)$ and $h_0(|v|)$, the flux $F(v,\tau)$ tends to zero everywhere. A separate transport equation for $F(x,\tau)$ can be derived from (2.32), but gives no useful simplifications.

We now turn to those properties of the transition kernel that emerge through the collision-number function $z(v)$. Since $h_0(v)$ is of even parity, it is clear from the relation (2.16) that

$$z(v) = 2\int_0^\infty \mathrm{d}u\max(|v|,u)\,h_0(u) = z(-v). \tag{2.34}$$

Hence immediately
$$z'(v) = 2\int_0^v \mathrm{d}u\, h_0(u), \tag{2.35}$$

and
$$z''(v) = 2h_0(v). \tag{2.36}$$

Alternatively, the last two properties follow by symbolic differentiation under the integral sign i.e., $d(|v|)/dv = \mathrm{sgn}\,(v)$ and $d^2(|v|)/dv^2 = 2\,\delta(v)$. Given the (full-range) normalization of $h_0(v)$ it is further evident that

$$z(v) \underset{v\to\pm\infty}{\sim} |v| \tag{2.37}$$

and, since $z'(\pm\infty) = 1$,

$$z(v) - vz'(v) \rightarrow 0; \quad v \rightarrow \pm\infty. \tag{2.38}$$

Thus in the scaling chosen $z(v)$ is a monotone increasing function, symmetrical about a minimum at $v = 0$ and behaving for small v as

$$z(v) = 1 + 2h_0(0)\,v^2 + O(v^4). \tag{2.39}$$

To these we may add the important bounds

$$1 \leqslant z(v) \leqslant 1 + |v|. \tag{2.40}$$

2.4. *The Maxwellian heat-bath*

To exemplify the scaling process and link up with our earlier work we shall briefly set out the above steps for the special case of the Maxwellian heat-bath. Let V be the real velocity of a heat-bath particle of mass M, Maxwell distributed at temperature T. The Maxwell distribution for one dimension is

$$H_0(V) = (M/2\pi k_B T)^{\frac{1}{2}} \exp\,(-MV^2/2k_B T), \tag{2.41}$$

with mean speed

$$V_0 = (2k_B T/\pi M)^{\frac{1}{2}}.$$

The transition kernel can thus be written

$$K(U, V) = C(2k_B T/\pi M)^{\frac{1}{2}}\,|U - V|\exp\,(-MV^2/2k_B T), \tag{2.42}$$

where C is the time-scaling factor as before. The collision-number function (2.3) can be evaluated as

$$Z(V) = C[V\,\mathrm{erf}\,(V/\pi^{\frac{1}{2}}V_0) + V_0 \exp -(V^2/\pi V_0^2)]. \tag{2.43}$$

Following our previous scaling procedure with V_0 as above, we arrive at the dimensionless quantities

$$h_0(v) = \pi^{-1}\exp\,(-v^2/\pi), \tag{2.44}$$

$$k(u, v) = \pi^{-1}\,|u - v|\exp\,(-v^2/\pi), \tag{2.45}$$

$$z(v) = v\,\mathrm{erf}\,(v/\pi^{\frac{1}{2}}) + \exp\,(-v^2/\pi). \tag{2.46}$$

Noting that $z'(v) = \mathrm{erf}\,(v/\pi^{\frac{1}{2}})$ we see that the Maxwellian heat-bath distribution satisfies the special relation

$$z(v) = vz'(v) + \tfrac{1}{2}\pi z''(v). \tag{2.47}$$

In general this is true only asymptotically (cf. equation (2.38)). A representation of the symmetric kernel (2.18) is drawn in figure 3, and the collision number function $z(x)$ is shown in figure 4, both for the Maxwellian heat-bath.†

† In our earlier publications (Hoare & Rahman 1973, 1974, Barker *et al.* 1977) we used the more convenient variable $x = V/V_0\pi^{\frac{1}{2}}$ with evident simplification of the above equations. We adhere to the choice $v = V/V_0$ in the present work rather than carry stray factors of $\pi^{\frac{1}{2}}$ through the whole of our general development.

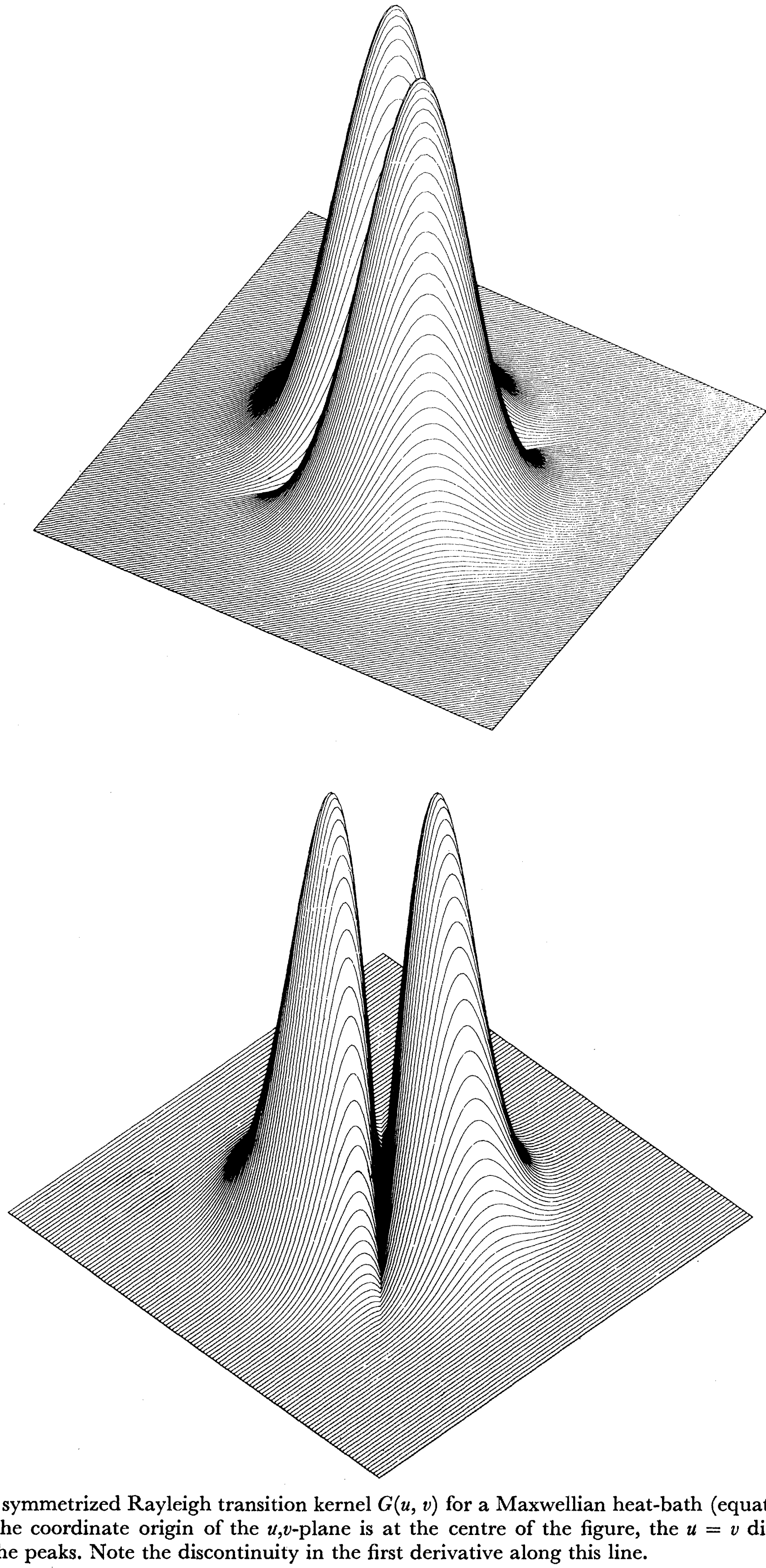

FIGURE 3. The symmetrized Rayleigh transition kernel $G(u, v)$ for a Maxwellian heat-bath (equations (2.18) and (2.45)). The coordinate origin of the u,v-plane is at the centre of the figure, the $u = v$ diagonal running between the peaks. Note the discontinuity in the first derivative along this line.

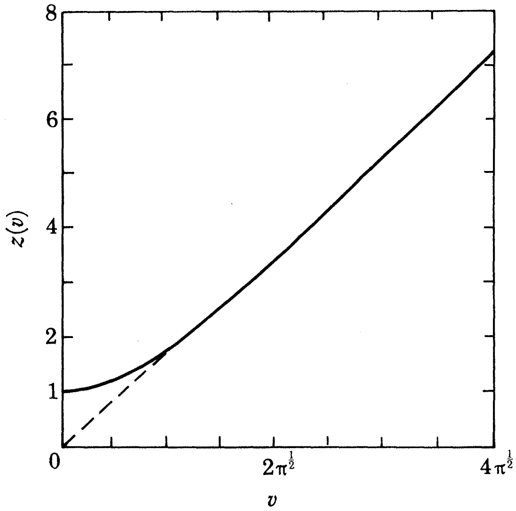

FIGURE 4. The collision-number function $z(v) = v \operatorname{erf}(v/\pi^{\frac{1}{2}}) + \exp(-v^2/\pi)$ for the Rayleigh test-particle in a Maxwellian heat-bath (equation (2.46)). The asymptote $z(v) \sim v$ is shown as a dashed line.

3. Spectral properties and the eigenvalue solution

As is now well established in particle transport theory (Williams 1966, 1971) the general solution of equation (2.5) can be formally expressed as

$$p(v,\tau) = h_0(v)\left[1 + \sum_k a_k \phi_k(v)\, e^{-\lambda_k \tau} + \int_{\lambda \in C} a(\lambda)\, \phi(v,\lambda)\, e^{-\lambda\tau}\, d\lambda\right]. \tag{3.1}$$

Here $\{\lambda_k\}$ is the discrete spectrum of the operator $\mathscr{A}$ of equation (2.7) and C represents the continuous spectrum with values $\lambda \in [1, \infty]$ in our present scaling. The eigenfunctions $\phi_k(v)$ and $\phi(v, \lambda)$ satisfy

$$\mathscr{A}\phi = \lambda\phi, \tag{3.2}$$

with λ in the discretum and continuum respectively. The equilibrium distribution arises from the special eigenvalue $\lambda_0 = 0$ with eigenfunction $\phi_0(v) = h_0(v)$ according to (2.17). The quantities a_k and $a(\lambda)$ are functions of the discrete and continuous variable λ to be determined from the given initial conditions $p(v, 0)$.

The eigenvalue problem may be seen explicitly if we separate the variables as

$$p(v,\tau) = h_0(v)\,\phi(v)\,\Theta(\tau) \tag{3.3}$$

and substitute in (2.5). In this way we arrive at the conditions

$$\phi(v,\lambda) = \frac{1}{[z(v)-\lambda]}\int_{-\infty}^{\infty} |u-v|\, h_0(u)\, \phi(u)\, du, \tag{3.4}$$

$$\Theta(\tau) = e^{-\lambda\tau}, \tag{3.5}$$

with λ the separation constant.

In equation (3.4) we see how the continuous spectrum is associated with the vanishing of the denominator, $z(v) - \lambda$, which, referring back to (2.39), we may confirm occurs when $z(0) = 1 \leqslant \lambda \leqslant \infty$. That the continuum is real and positive is self-evident; for the discretum we may prove that $\mathscr{A}$ is positive-definite by noting that, for arbitrary $g(v) \in L_2(-\infty, +\infty)$, we have, on using (2.17) and (2.18),

$$(gh_0^{-\frac{1}{2}}, \mathscr{A}gh_0^{\frac{1}{2}}) = \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}u \int_{-\infty}^{\infty} \mathrm{d}v |u-v| \, [g(u)\, h_0(v)^{\frac{1}{2}} - g(v)\, h_0(u)^{\frac{1}{2}}]^2$$
$$\geqslant 0.$$

We can now usefully separate the parity components of ϕ, obtaining the uncoupled equations

$$[z(v)-\lambda]\,\phi_{\mathrm{ev}}(v,\lambda) = 2\int_0^{\infty} \mathrm{d}u \max(|v|, u)\, h_0(u)\, \phi_{\mathrm{ev}}(u,\lambda), \tag{3.6}$$

$$[z(v)-\lambda]\,\phi_{\mathrm{od}}(v,\lambda) = -2\,\mathrm{sgn}\,(v)\int_0^{\infty} \mathrm{d}u \min(|v|, u)\, h_0(u)\, \phi_{\mathrm{od}}(u,\lambda). \tag{3.7}$$

From the definition of $z(v)$ and its even parity, it is evident that the eigenvalue $\lambda_0 = 0$ and the equilibrium eigenfunction $\phi_0(v) = 1$ belong to the *even* parity equation.

It will be clear that there is much more to the implementation of equation (3.1) as a useful solution than the simple Fourier analysis required for a regular eigenvalue problem. In brief, we must first establish the correct interpretation of the singular eigenfunctions $\phi(v, \lambda)$, prove normalization and completeness for an adequate class of initial distributions $p(v, 0)$, and then give a clear prescription for the determination of the expansion coefficients $a(\lambda)$. The general background to this problem has been discussed by Case (1959, 1960) and evaluated critically by Hangelbroek (1973); here we shall illustrate in technical detail the implementation of the 'singular eigenfunction method' by reference to the Rayleigh model. It will be convenient to consider in turn the discrete spectrum, then the even and odd singular eigenfunctions, and then finally to derive expressions for the expansion coefficients after completeness has been proved.

3.1. *The discrete spectrum*

On differentiating equation (3.4) with respect to v, we obtain first the integro-differential equation

$$z'(v)\,\phi(v,\lambda) + \phi'(v,\lambda)\,[z(v)-\lambda] = \int_{-\infty}^{\infty} \mathrm{d}u\,\mathrm{sgn}\,(v-u)\, h_0(u)\, \phi(u,\lambda), \tag{3.8}$$

and then the singular second-order equation

$$[z(v)-\lambda]\,\phi''(v,\lambda) + 2z'(v)\,\phi'(v,\lambda) = 0. \tag{3.9}$$

Note that the latter is obtained by differentiation of either of the parity components (3.6) or (3.7), this confirming that the respective parities are accounted for in the boundary conditions of the problem. Now, so long as $\lambda < 1$, this is an elementary, regular equation whose general solution is the linear combination

$$\phi(v,\lambda) = A(\lambda)\int_0^v \frac{\mathrm{d}y}{[z(y)-\lambda]^2} + B(\lambda). \tag{3.10}$$

Here A and B are as yet arbitrary functions of λ. It is convenient now to put $v = 0$ in (3.6) and (3.7), and we observe that

$$(1-\lambda)\,\phi(0,\lambda) = \int_{-\infty}^{\infty} \mathrm{d}u\,|u|\, h_0(u)\, \phi(u,\lambda), \tag{3.11}$$

$$(1-\lambda)\,\phi'(0,\lambda) = -\int_{-\infty}^{\infty} \mathrm{d}u\,\mathrm{sgn}\,(u)\, h_0(u)\, \phi(u,\lambda). \tag{3.12}$$

Recognizing that the terms in A and B in (3.10) are the *even* and *odd* components of the solution respectively, we may form the conditions

$$(1-\lambda)\,B = B, \tag{3.13}$$

and

$$\frac{A}{1-\lambda} = \frac{A}{1-\lambda} - A\int_0^\infty \frac{\mathrm{d}y}{[z(y)-\lambda]^2}. \tag{3.14}$$

Here we have used the important relation

$$2\int_0^\infty \mathrm{d}y\, h_0(y)\int_0^y \frac{\mathrm{d}w}{[z(w)-\lambda]^2} = \int_0^\infty \frac{\mathrm{d}y}{[z(y)-\lambda]^2} - \frac{1}{1-\lambda}, \tag{3.15}$$

this being the first of many occasions where the properties $z''(v) = 2h_0(v)$ and $z'(\infty) = 1$ will allow us to simplify by partial integration (see Appendix 2).

From the above it follows immediately that *either* $\lambda = 0$, in which case $A = 0$ and B is arbitrary, *or* $\lambda \neq 0$, when necessarily $A = B = 0$. No other possibilities exist. Thus, with the exception of the single equilibrium eigenvalue $\lambda = 0$, *the discretum is empty*. This confirms for the general heat-bath the result obtained by Hoare & Rahman (1974) for the Maxwellian. A more abstract proof of the same result has recently been given by Dreissler (1981).

3.2. *The singular eigenfunctions*

As we have outlined previously (Hoare 1971, Hoare & Rahman 1974) the solutions of equations (3.6) or (3.7), while radically altered in the continuum range $\lambda > 1$, may nevertheless be treated satisfactorily within the realm of generalized functions. Recalling that the generalized solution to

$$x^n F(x) = 1$$

is

$$F(x) = \mathrm{Pf}\,x^{-n} + \sum_{k=0}^{n-1} a_k \delta^{(k)}(x), \tag{3.16}$$

with $\delta^{(n)}(x)$ the derivatives of the δ-function and $\mathrm{Pf}\,x^{-n}$ the inverse-power 'pseudofunction' (Zemanian 1965, § 1.4), we may reinterpret the first integral of equation (3.9) in the following way. Writing it in the more compact form

$$(\mathrm{d}/\mathrm{d}v)\,\{[z(v)-\lambda]^2\phi(v,\lambda)\} = 0, \tag{3.17}$$

in which $\phi(v)$ can stand for either the full eigenfunction or one of its parity components, we appeal to the result that, if $G(x)$ is a distribution, then the equation $G'(x) = 0$ has only the solution $G(x) = \text{const.}$, i.e. the classical one (see for example Jones 1966, p. 89). Thus it follows that there are two first integrals

$$[z(v)-\lambda]^2\,\phi'_{\mathrm{ev}}(v,\lambda) = A_1(\lambda) \tag{3.18}$$

and

$$[z(v)-\lambda]^2\,\phi'_{\mathrm{od}}(v,\lambda) = A_2(\lambda), \tag{3.19}$$

with the functions $A_1(\lambda)$, $A_2(\lambda)$ to be determined through the original integral equation. We can now examine the two parity types separately.

Since undoubtedly $\phi'_{\mathrm{ev}}(v,\lambda)$ is an *odd* function, we recognize that the constant A_1 can only be zero and that the first integral can be written

$$\phi'_{\mathrm{ev}}(v,\lambda) = B_1[\delta(v-|v_\lambda|) - \delta(v+|v_\lambda|)] + C_1[\delta'(v-|v_\lambda|) + \delta'(v+|v_\lambda|)]. \tag{3.20}$$

Here we use the symbol v_λ for the root such that $z(v_\lambda) = \lambda$, noting in advance that we shall need the identity

$$\delta[z(v)-\lambda] = [z'(v_\lambda)]^{-1}\,\delta(v-v_\lambda). \tag{3.21}$$

It then follows on integration that

$$\phi_{\mathrm{ev}}(v,\lambda) = A + B_1[H(v-|v_\lambda|)+H(-v-|v_\lambda|)] + C_1[\delta(v-|v_\lambda|)+\delta(v+|v_\lambda|)], \tag{3.22}$$

where $H(.)$ represents the Heaviside unit step function and A, B_1 and C_1 are constants of integration, not of course independent. To obtain these we must substitute back into the original equation (3.6), its once-differentiated version (3.8) and the pure differential equation (3.9). It suffices, however, to take the $v = 0$ case from which we obtain

$$(1-\lambda)\,A = 2\int_0^\infty \mathrm{d}y\,h_0(y)\,\phi_{\mathrm{ev}}(y,\lambda) = A + B_1[\lambda - v_\lambda z'(v_\lambda)] + 2\,|v_\lambda|\,h_0(v_\lambda)\,C_1. \tag{3.23}$$

Finally,
$$B_1 z'(|v_\lambda|) = 2C_1 h_0(v_\lambda).$$

On solving in terms of the remaining unknown the even eigenfunctions become

$$\phi_{\mathrm{ev}}(v,\lambda) = A\{1 - H(v-|v_\lambda|) - H(-v-|v_\lambda|) + q(v_\lambda)\,[\delta(v-|v_\lambda|)+\delta(v+|v_\lambda|)]\}, \tag{3.24}$$

in which we have written
$$q(v_\lambda) = \tfrac{1}{2}\,|z'(v_\lambda)|/h_0(v_\lambda). \tag{3.25}$$

The remaining constant A must be supplied by a normalization.

Turning now to the *odd* eigenfunctions, we can proceed in a similar manner. Since $\phi'_{\mathrm{od}}(v,\lambda)$ is certainly of *even* parity, we must retain the pseudofunction term in (3.16) and select the even components of the δ-function and its derivative. Thus

$$\phi'_{\mathrm{od}}(v,\lambda) = A_2\,\mathrm{Pf}\,[z(v)-\lambda]^{-2} + B_2[\delta(v-|v_\lambda|)+\delta(v+|v_\lambda|)] + C_2[\delta'(v-|v_\lambda|)-\delta'(v+|v_\lambda|)].$$

On integrating this we obtain

$$\phi_{\mathrm{od}}(v,\lambda) = A_2 R(v_1\lambda) + B_2[H(v-|v_\lambda|) - H(-v-|v_\lambda|)] + C_2[\delta(v-|v_\lambda|)-\delta(v+|v_\lambda|)], \tag{3.26}$$

in which we have written $R(v,\lambda)$ for the Hadamard pseudofunction

$$R(v,\lambda) = \mathrm{Pf}\int_0^v \frac{\mathrm{d}y}{[z(y)-\lambda]^2}. \tag{3.27}$$

(See Appendix 3. We shall usually drop the prefix Pf when the singularity is clear from the context.) Two of the constants of integration can be eliminated as for the even eigenfunctions. If we put $v = 0$ in (3.7) it follows that

$$\frac{A_2}{1-\lambda} = -2A_2\int_0^\infty \mathrm{d}y\,h_0(y)\,R(y,\lambda) - 2B_2\int_{|v_\lambda|}^\infty \mathrm{d}y\,h_0(y) - 2C_2\,h_0(v_\lambda), \tag{3.28}$$

which may be used in combination with equation (3.17). After a similar development to that for equation (3.23) we find

$$B_2 z'(|v_\lambda|) = \tfrac{1}{2}C_2 h_0(v_\lambda). \tag{3.29}$$

Lastly, using the singular counterpart of (3.15),

$$2\int_0^\infty \mathrm{d}y\,h_0(y)\,R(y,\lambda) = R(\infty,\lambda) - \frac{1}{(1-\lambda)}. \tag{3.30}$$

(see Appendix 2), we can reduce equation (3.28) to

$$-A_2 R(\infty, \lambda) = B_2[1 - z'(|v_\lambda|)] + 2C_2 h_0(v_\lambda).$$

Thus, on solving in terms of A_2, the odd solution becomes

$$\phi_{\mathrm{od}}(v, \lambda) = A_2\{R(v, \lambda) - R(\infty, \lambda)\,[H(v - |v_\lambda|) - H(-v - |v_\lambda|)] \\ - R(\infty, \lambda)\, q(v_\lambda)\,[\delta(v - |v_\lambda|) - \delta(v + |v_\lambda|)]\}. \tag{3.31}$$

Again the remaining constant is to be determined by a normalization.

It may be as well to recall here that the action of the pseudofunctions $\mathrm{Pf}[z(x) - \lambda]^{-2}$ and $R(x, \lambda)$ is determined through the functional

$$\langle \mathrm{Pf}\, G(x), \varphi(x)\rangle = \mathrm{Fp}\int_{-\infty}^{\infty} \mathrm{d}x\, G(x)\, \varphi(x),$$

in which $G(x)$ is the given function and $\phi(x)$ is an appropriate testing function. The operation indicated by Fp on the right means the extraction of the Hadamard finite part of a formally divergent integral, in effect the expansion of the integrand about the singularity in sufficient order to isolate regular and singular contributions, followed by subtraction of the latter. Operation with $\mathrm{Pf}\, R(v, \lambda)$ involves double integrals, but this is no essential complication. For further details of the extraction of finite parts and the properties of the function $R(v, \lambda)$, refer to Appendix 3.

3.2.1. *Orthogonality of the eigenfunctions*

The orthogonality of the eigenfunctions of the transition operator for the Rayleigh problem is in effect guaranteed by the symmetry of the operator $\mathscr{G}$ defined in equation (2.18) which derives in turn from the detailed-balance condition (2.12). Nevertheless it is instructive to confirm the orthogonality property directly, while at the same time finding the normalization functions that will be needed for Fourier analysis.

If we define the inner product

$$(\phi_A(\lambda), \phi_B(\lambda')) = \int_{-\infty}^{\infty} \mathrm{d}y\, h_0(y)\, \phi_A(y, \lambda)\, \phi_B(y, \lambda), \tag{3.32}$$

in which A and B may stand for any of the designations '0', 'ev' or 'od' then it is clear on parity grounds that

$$(\phi_0(\lambda), \phi_{\mathrm{od}}(\lambda')) = 0, \tag{3.33}$$

and

$$(\phi_{\mathrm{ev}}(\lambda), \phi_{\mathrm{od}}(\lambda')) = 0. \tag{3.34}$$

It remains to prove that

$$(\phi_0(\lambda), \phi_{\mathrm{ev}}(\lambda')) = 0, \tag{3.35}$$

and that $(\phi_{\mathrm{ev}}(\lambda), \phi_{\mathrm{ev}}(\lambda'))$ and $(\phi_{\mathrm{od}}(\lambda), \phi_{\mathrm{od}}(\lambda'))$ are of the form

$$(\phi_{\mathrm{ev}}(\lambda), \phi_{\mathrm{ev}}(\lambda')) = A_1(\lambda)^2 N_1(\lambda)\, \delta(\lambda - \lambda'), \tag{3.36}$$

and

$$(\phi_{\mathrm{od}}(\lambda), \phi_{\mathrm{od}}(\lambda')) = A_2(\lambda)^2 N_2(\lambda)\, \delta(\lambda - \lambda'), \tag{3.37}$$

respectively, with $N_1(\lambda)$, $N_2(\lambda)$ explicit normalization functions.

The first of these combinations is straightforward since, by partial integration, we have

$$(\phi_0, \phi_{\mathrm{ev}}(\lambda)) = \int_{-\infty}^{\infty} \mathrm{d}v\, h_0(v)\, \phi_{\mathrm{ev}}(v, \lambda) \\ = A(\lambda)\left[2\int_0^{|v_\lambda|} \mathrm{d}y\, h_0(y) - z'(|v_\lambda|)\right] = 0. \tag{3.38}$$

Turning next to the *even*, singular subset we now examine the integral (3.36), assuming with no loss of generality that $\lambda' \leqslant \lambda$, i.e. that $0 \leqslant v_{\lambda'} \leqslant v_\lambda$. The following identities for the step and δ-functions will be needed:

$$[H(x-|a|)-H(x+|a|)][\delta(x-|b|)+\delta(x+|b|)] = H(|a|-|b|)[\delta(x-|b|)+\delta(x+|b|)], \qquad (3.39)$$

$$-[H(x-|a|)-H(x+|a|)][H(x-|b|)-H(x+|b|)] = H(x-\max(|a|,|b|))-H(x+\max(|a|,|b|)). \qquad (3.40)$$

Using these we see that the range of integration can be split into four:

$$\int_{-\infty}^{\infty} \equiv \int_{-\infty}^{-v_\lambda} + \int_{-v_\lambda}^{-v_{\lambda'}} + \int_{-v_{\lambda'}}^{v_\lambda} + \int_{v_\lambda}^{\infty}.$$

On careful examination of each resulting group of terms we find that the expected cancellations occur and, after reverting to the λ- rather than the v_λ-variable, we find the only surviving term to be a convolution of δs, from which

$$(\phi_{\mathrm{ev}}(v,\lambda), \phi_{\mathrm{ev}}(v,\lambda')) = [z'(|v_\lambda|)^3/2h_0(v_\lambda)]\, A_1(\lambda)^2\, \delta(\lambda-\lambda'). \qquad (3.41)$$

We have thus proved the normalization function to be

$$N_1(\lambda) = [z'(|v_\lambda|)^3/2h_0(v_\lambda)]\, A_1(\lambda), \qquad (3.42)$$

the constant $A_1(\lambda)$ being still disposable. If we wish for an orthonormal set, we can evidently create it by setting

$$A_1(\lambda) = \left[\frac{2h_0(v_\lambda)}{z'(|v_\lambda|)^3}\right]^{\frac{1}{2}} = 2h_0(v_\lambda)^{\frac{1}{2}}\left[\int_0^{v_\lambda} h_0(y)\,\mathrm{d}y\right]^{-\frac{3}{2}}. \qquad (3.43)$$

The proof of orthogonality for the *odd* eigenfunctions is more problematic. Composing the integral (3.37) we find that it breaks down into six terms containing the possible combinations of $H(.)$, $\delta(.)$ and $R(.)$ in the products of the expressions (3.26). To simplify these we need the further identities

$$[H(x-|a|)-H(-x-|a|)][\delta(x-|b|)-\delta(x+|b|] = H(|b|-|a|)[\delta(x-|b|)+\delta(x+|b|)], \qquad (3.44)$$

$$[H(x-|a|)-H(-x-|a|)][H(x-|b|)-H(-x-|b|)] = H(x-\max(|a|,|b|))+H(-x-\max(|a|,|b|)), \qquad (3.45)$$

and the easily demonstrated integrals

$$2\int_0^{\infty} \mathrm{d}y\, R(y,\lambda)\, R(y,\lambda')\, h_0(y) = R(\infty,\lambda)\, R(\infty,\lambda') - [R(\infty,\lambda)-R(\infty,\lambda')]/(\lambda-\lambda'), \qquad (3.46)$$

and

$$2\int_{|v_\lambda|}^{\infty} \mathrm{d}y\, h_0(y)\, R(y,\lambda') = R(\infty,\lambda) - z'(|v_\lambda|)\, R(|v_\lambda|,\lambda') - \frac{1}{\lambda-\lambda'} \qquad (3.47)$$

(Appendix 3). It follows after lengthy manipulations that

$$(\phi_{\mathrm{od}}(v,\lambda), \phi_{\mathrm{od}}(v,\lambda')) = [A_2(\lambda)^2 R(\infty,\lambda)^2 z'(|v_\lambda|)^3/2h_0(v_\lambda)]\, \delta(\lambda-\lambda'). \qquad (3.48)$$

Thus the required normalization constant is

$$N_2(\lambda) = R(\infty,\lambda)^2 z'(|v_\lambda|)^3/2h_0(v_\lambda) = R(\infty,\lambda)^2 N_1(\lambda). \qquad (3.49)$$

3.3. *Completeness*

The problem of completeness and the associated Fourier analysis of a probability distribution $P(v, \tau)$ is one of some subtlety. Indeed it seems to be characteristic of model transport theory that, in the rare instances where exact solutions are known, the precise nature of the space spanned by the singular eigenfunctions remains obscure, the determination of the expansion coefficients requires careful analysis and each case must be treated very much on its own merits. For further detail of background and techniques in this controversial area we can only refer again to Case & Zweifel (1967) and Hangelbroek (1973).

Here we shall evade the more general issues and concentrate on a constructive proof of the completeness of the even and odd eigenfunction sets for the Rayleigh model with respect to a function space adequate for the problem in hand. As usual in particle transport theory it will be sufficient to require that we span a space of 'reasonable' initial distributions $P(v, \tau)$ for example those for which $p(v, \tau)$ possesses a Laplace transform (cf. Corngold *et al.* 1963). In one dimension a satisfactory characterization might be the space $L_p(-\infty, +\infty)$ with $p > 1$, augmented by δ-functions. Ronen (1973) has usefully discussed this and other aspects of the choice of function spaces relevant to transport processes.

We shall first give a constructive proof of the completeness of the *even* eigenfunctions, this being relatively straightforward. We then outline a non-constructive proof of completeness for the *odd* functions similiar to that of Hoare & Rahman (1974) for the Maxwellian case but leave a fuller exposé of this problem to be treated under the heading of the Laplace transform method in § 4. Finally the more practical problem of obtaining the expansion coefficients $a(\lambda)$ for use in equation (3.1) is taken up.

3.3.1. *Completeness of the even eigenfunctions*

Let $\mathscr{D}_1$ be the (as yet uncharacterized) function space spanned by the functions ϕ_{ev} with weight $h_0(v)$. Since in the initial-value problem we expect an evolution $p(v, \tau) \to p(v, \infty) = h_0(v)$ to occur, it is reasonable to restrict attention to the *even* component of p orthogonal to $h_0(v)$.

Consider a function $\zeta(v) \in \mathscr{D}_1$ with this property. Then we may assert that, for suitable expansion coefficients $a(\lambda)$,

$$\zeta(v) = h_0(v)\left[1 + \int_1^\infty \mathrm{d}\lambda\, a(\lambda)\, \phi_{\mathrm{ev}}(v, \lambda)\right], \tag{3.50}$$

where necessarily

$$\int_{-\infty}^{\infty} \mathrm{d}v[\zeta(v) - h_0(v)] = 0. \tag{3.51}$$

On changing dependent variables, $f(v) = \zeta(v)/h_0(v)$, $\omega_1(v_\lambda) = A(v_\lambda)\, a(v_\lambda)$, and the independent variable $\lambda \to v_\lambda$, and inserting the expression (3.24) for ϕ_{ev}, the integral on the right of (3.50) yields

$$f(v) = \int_{|v|}^{\infty} \mathrm{d}v_\lambda\, \omega_1(v_\lambda)\, z'(v_\lambda) - \frac{z'(v)\, \omega_1(v)}{2h_0(v)} + 1. \tag{3.52}$$

From this, on differentiation with respect to v, the following equation emerges:

$$\mathrm{d}\omega_1(v)/\mathrm{d}v + P(v)\, \omega_1(v) = Q(v), \tag{3.53}$$

in which

$$P(v) = (\mathrm{d}/\mathrm{d}v)\{\ln[z'(|v|)^3/2h_0(v)]\}, \tag{3.54}$$

and

$$Q(v) = -2f'(v)\, h_0(v)/z'(v)^2. \tag{3.55}$$

The solution follows in the usual way as

$$\omega_1(v) = \frac{2h_0(v)}{z'(|v|)^3}\left[2\int_0^{|v|} h_0(y) f(y)\,\mathrm{d}y - z'(v) f(v) + \beta\right],$$

in which β is a constant of integration. This is in fact zero, as may be shown on substitution back into equation (3.52). Finally

$$\omega_1(v) = \frac{2h_0(v)}{z'(|v|)^3}\left[2\int_0^{|v|} \zeta(y)\,\mathrm{d}y - \frac{z'(v)}{h_0(v)}\right]. \tag{3.56}$$

We have thus found a constructive procedure for determining $a(v)$ under only the mildest conditions on the function $\zeta(v)$: no more than simple integrability is required.

Now suppose that we seek an alternative derivation by the 'naïve' method of using orthogonality under the assumption *pro tem.* that the necessary integrals can be interchanged. With the use of the normalization (3.95) it then follows immediately that

$$\begin{aligned}\int_{-\infty}^{\infty} \mathrm{d}v\, \zeta(v)\, \phi_{\mathrm{ev}}(v,\lambda) &= \int_{-\infty}^{\infty} \mathrm{d}v\, \phi_{\mathrm{ev}}(v,\lambda)\, h_0(v) \int_1^{\infty} \mathrm{d}\lambda'\, a(\lambda')\, \phi_{\mathrm{ev}}(v,\lambda') \\ &\overset{?}{=} \int_1^{\infty} \mathrm{d}\lambda'\, a(\lambda') \int_{-\infty}^{\infty} \mathrm{d}v\, h_0(v)\, \phi_{\mathrm{ev}}(v,\lambda)\, \phi_{\mathrm{ev}}(v,\lambda') \\ &= A(\lambda)^2 N_1(\lambda)\, a(\lambda).\end{aligned}$$

If now the left-hand side is evaluated by using the expression (3.24) for ϕ_{ev}, the result corresponding to equation (3.56) is recovered. This provides *post hoc* justification for the interchange of integrations and the use of the 'natural' Fourier coefficient formula

$$a(\lambda) = \frac{1}{N_1(\lambda)\, A(\lambda)^2}\int_{-\infty}^{\infty} \mathrm{d}v\, \zeta_1(v)\, \phi_{\mathrm{ev}}(v,\lambda) \tag{3.57}$$

so far as the *even* functions are concerned.

3.3.2. *Completeness of the odd eigenfunctions*

The completeness problem for the *odd* eigenfunctions is by no means as straightforward as that for the even and the caution with which we approached the latter will be seen to be fully justified. Although a much neater approach to completeness will be possible with the aid of the Laplace transform method of § 4, a direct method is still of interest in exposing some of the technical problems associated with the Hadamard pseudofunctions $R(v,\lambda)$.

Since the eigenfunction $\phi_0 = h_0$ is purely *even*, we can assert the existence of a function space $\mathscr{D}_{\mathrm{od}}$ spanned by the ϕ_{od} and a class of functions $\zeta_2(v)$ (not in general probability distributions) such that, for $\zeta_2 \in \mathscr{D}_{\mathrm{od}}$, there exist expansions of the form

$$\zeta_2(v) = h_0(v) \int_1^{\infty} \mathrm{d}\lambda\, b(\lambda)\, \phi_{\mathrm{od}}(v,\lambda). \tag{3.58}$$

Entering the expression (3.26) for the odd eigenfunctions and rearranging the result slightly we find that

$$\begin{aligned}\zeta_2(v) = h_0(v)\int_0^{\infty} \mathrm{d}v_\lambda\, \omega_2(v_\lambda)\, z'(v_\lambda)\, R(v,\lambda) \\ -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}v}\left[z'(|v|)\int_0^{|v|} \mathrm{d}v_\lambda\, R(\infty, z(v_\lambda))\, \omega_2(v_\lambda)\right],\end{aligned}$$

in which we have put $\omega_2(\lambda) = A_2(\lambda)\, b(\lambda)$ and written the pseudofunction $R(v,\lambda)$ as $R(v, z(v_\lambda))$ for the sake of integration over v_λ. By direct integration it then follows that

$$\int_{-\infty}^{v} \mathrm{d}y\, \zeta_2(y) = \int_{-\infty}^{v} \mathrm{d}y\, h_0(y) \int_0^\infty \mathrm{d}v_\lambda\, \omega_2(v_\lambda)\, z'(v_\lambda)\, R(y, z(v_\lambda))$$
$$+\frac{1}{2}\int_0^\infty \mathrm{d}v_\lambda\, w_2(v_\lambda)\, R(\infty, z(v_\lambda)) - \tfrac{1}{2}z'(|v|)\int_0^{|v|} \mathrm{d}v_\lambda\, \omega_2(v_\lambda)\, z'(v_\lambda)\, R(\infty, z(v_\lambda)). \quad (3.59)$$

In all these expressions we leave it understood that the quantities $R(.,.)$ are pseudofunctions and that the Hadamard finite parts are taken as appropriate. The double integrals arising will not in general be interchangable; however, a sufficient condition for them to be so is that $\zeta_2(v_\lambda)$ satisfy a Lipschitz condition (see for example Muskhelishvili 1953). With this proviso we can reverse the integral signs in the first term on the right and simplify it as follows:

$$\int_0^\infty \mathrm{d}v_\lambda\, \omega_2(v_\lambda)\, z'(v_\lambda) \int_{-\infty}^{v} \mathrm{d}y\, h_0(y)\, R(y, z(v_\lambda))$$
$$= \tfrac{1}{2}z'(v)\int_0^\infty \mathrm{d}v_\lambda\, \omega_2(v_\lambda)\, z'(v_\lambda)\, R(v, z(v_\lambda)) + \frac{1}{2}\int_0^\infty \mathrm{d}v_\lambda\, \omega_2(v_\lambda)\, z'(v_\lambda)\, R(\infty, z(v_\lambda))$$
$$+\,\mathrm{Pv}\int_0^\infty \frac{\mathrm{d}v_\lambda\, \omega_2(v_\lambda)\, z'(v_\lambda)}{[z(v) - z(v_\lambda)]}.$$

Here the Cauchy principal value, Pv, arises for the first time through the identity

$$\mathrm{Pv}(1/x) = \mathrm{Pf}\, H(x)/x = \mathrm{Pf}\, H(-x)/x \quad (3.60)$$

(cf. Zemanian 1965, § 1.4).

Putting this result back into equation (3.59) we arrive by further manipulations not at an explicit expression for $\omega_2(v_\lambda)$ comparable with (3.56) but to a singular integral equation to be solved for the unknown function. This takes the form

$$\frac{z'(|v|)^3 R(\infty, v)\, \omega_2(v)}{2h_0(v)} - \mathrm{Pv}\int_0^\infty \frac{\mathrm{d}v_\lambda\, \omega_2(v_\lambda)\, z'(v_\lambda)}{z(v) - z(v_\lambda)} = 2\int_{-\infty}^{v} \mathrm{d}y\, \zeta_2(y) - \frac{z'(v)\, \omega_2(v)}{h_0(v)}. \quad (3.61)$$

This is a standard equation of Carleman type for which a formal solution can be written via a Hilbert transform. Here we need only the existence of the solution under the stated conditions; for full details and background refer to Tricomi (1975). With the above, we have demonstrated the completeness of the set $\{\phi_{\mathrm{od}}(v)\}$, albeit in a non-constructive manner. Further insight into the behaviour of the singular basis sets will be gained in the next section, in which we study the Fourier expansion procedure for the same.

3.4. *Derivation of the expansion coefficients*

If we attempt to find the expansion coefficients $b(\lambda)$ of (3.58) by evaluation of the integrals

$$\int_{-\infty}^{\infty} \mathrm{d}v\, \zeta_2(v)\, \phi_{\mathrm{od}}(v,\lambda) = \int_{-\infty}^{\infty} \mathrm{d}v\, h_0(v)\, \phi_{\mathrm{od}}(v,\lambda) \int_1^\infty \mathrm{d}\lambda'\, \phi_{\mathrm{od}}(v,\lambda') \quad (3.62)$$

using orthogonality, then there can be no question of interchanging the operations on the right in view of the pseudofunctions that appear there. To see what is involved let us abbreviate the functions ϕ_{od} in a form, the usefulness of which will become clear as we go on. We put

$$\phi_{od}(v,\lambda) = A_2(\lambda)\,[R(v,\lambda)-\alpha(v,\lambda)], \tag{3.63}$$

$$\alpha(v,\lambda) = R(\infty,\lambda)\,g(v,\lambda)/g(\infty,\lambda), \tag{3.64}$$

$$g(\infty,\lambda) = 2h_0(v_\lambda)/z'(|v_\lambda|)^3, \tag{3.65}$$

$$g(v,\lambda) = g(\infty,\lambda)\,\{[H(v-|v_\lambda|)-H(-v-|v_\lambda|)]+z'(v_\lambda)\,[\delta(v-|v_\lambda|)-\delta(v+|v_\lambda|)]\}, \tag{3.66}$$

noting that the function $g(v,\lambda)$ is an explicit form for the definite integral

$$g(v,\lambda) = \int_0^v \mathrm{d}y\,\delta'[z(y)-\lambda]. \tag{3.67}$$

Examining now the right-hand side of (3.62) we see that this may be written

$$\int_{-\infty}^{\infty}\mathrm{d}v\,\zeta_2(v)\,\phi_{od}(v,\lambda) = \beta_1(\lambda)+\beta_2(\lambda),$$

where $\beta_1(\lambda)$ and $\beta_2(\lambda)$ are the integrals

$$\beta_1(\lambda) = A_2(\lambda)\int_{-\infty}^{\infty}\mathrm{d}v\,h_0(v)\,R(v,\lambda)\int_0^1\mathrm{d}\lambda'\,A_2(\lambda')\,b(\lambda')\,R(v,\lambda'),$$

$$\beta_2(\lambda) = A_2(\lambda)\int_0^1\mathrm{d}\lambda'\,b(\lambda')\,A_2(\lambda')\int_{-\infty}^{\infty}\mathrm{d}v\,h_0(v)\,[\alpha(v,\lambda)\,\alpha(v,\lambda')-\alpha(v,\lambda)\,R(v,\lambda')-\alpha(v,\lambda')\,R(v,\lambda)].$$

Now, while the order of integration in the first integral can undoubtedly be reversed under mild conditions similar to those governing the ϕ_{ev}-integrals, the presence of the pseudofunctions locates the difficulty in $\beta_2(\lambda)$. But, although this type of double integral is unfamiliar, we know that a simple modification suffices to reduce the action of $R(v,\lambda)$ to the taking of Cauchy principal values (see Appendix 3). By transforming in this way we are then able to apply the Hardy–Poincaré–Bertrand formula to effect the interchange (Hardy 1908, Tricomi 1957). The theorem in its more general form states that

$$\mathrm{Pv}\int\frac{\mathrm{d}x}{x-y}\,\mathrm{Pv}\int\frac{\mathrm{d}y\,F(x,y,z)}{x-z} = \mathrm{Pv}\int\mathrm{d}y\,\mathrm{Pv}\int\frac{\mathrm{d}x\,F(x,y,z)}{(x-y)\,(x-z)}+\pi^2F(z,z,z). \tag{3.68}$$

Thus, as a result of the interchange of integral signs, the additional term $\pi^2F(z,z,z)$ must be entered.

In the present case we proceed as follows. The pseudofunction $R(v,\lambda)$ is decomposed by writing

$$R(v,\lambda) = R_{\mathrm{reg}}(v,\lambda)+R_{\mathrm{sing}}(v,\lambda), \tag{3.69}$$

in which (see Appendix 3, equation (A 3.7))

$$R_{\mathrm{reg}}(v,\lambda) = \mathrm{sgn}\,(v)\int_0^{|v|}\mathrm{d}u\left\{\frac{1}{[z(u)-z(v_\lambda)]^2}-\frac{1}{z'(v_\lambda)^2\,(u-v_\lambda)^2}\right\}, \tag{3.70}$$

$$R_{\mathrm{sing}}(v,\lambda) = \frac{-\mathrm{sgn}\,(v)}{z'(v_\lambda)^2}\,\mathrm{Pf}\int_0^{|v|}\frac{\mathrm{d}u}{[u-v_\lambda]^2}$$

$$= \frac{\mathrm{sgn}\,(v)}{z'(v_\lambda)^2}\,\mathrm{Pv}\left[\frac{1}{|v|-|v_\lambda|}\right]+\frac{\mathrm{sgn}\,(v)}{z'(v_\lambda)^2\,v_\lambda}. \tag{3.70}$$

The Poincaré–Bertrand integral is now narrowed down to one involving just the singular part of R. This is

$$I(\lambda) = A_2(\lambda)\,\mathrm{Pv}\int_{-\infty}^{\infty}\frac{\mathrm{d}v\,h_0(v)}{(|v|-|v_\lambda|)z'(v_\lambda)^2}\,\mathrm{Pv}\int_{-\infty}^{\infty}\frac{\mathrm{d}v_{\lambda'}\,A_2(v_\lambda)}{(|v|-|v_{\lambda'}|)\,z(v_{\lambda'})}.$$

Appeal to the theorem then allows us to write

$$I(\lambda) = A_2(\lambda)\,\mathrm{Pv}\int_0^{\infty}\frac{\mathrm{d}v}{v-v_\lambda}\,\mathrm{Pv}\int_0^{\infty}\frac{\mathrm{d}v_{\lambda'}\,A_2(\lambda')\,b(\lambda')\,h_0(v)}{(v-v_\lambda)\,(v-v_{\lambda'})\,z'(v_{\lambda'})\,z'(v_\lambda)^2}$$
$$= A_2(\lambda)\,\mathrm{Pv}\int_0^{\infty}\mathrm{d}v_\lambda\,\mathrm{Pv}\int_0^{\infty}\mathrm{d}v\,\frac{A_2(\lambda')\,b(\lambda')\,h_0(v)}{(v-v_\lambda)\,(v-v_{\lambda'})\,z'(v_{\lambda'})\,z'(v_\lambda)^2}$$
$$+\frac{2\pi^2\,b(\lambda)\,A_2(\lambda)^2\,h_0(v_\lambda)}{z'(|v_\lambda|)^3}. \tag{3.72}$$

The result is that

$$\int_{-\infty}^{\infty}\mathrm{d}v\,\zeta_2(v)\,\phi_{\mathrm{od}}(v,\lambda) = A_2(\lambda)^2\,b(\lambda)\,[N_2(\lambda)+2\pi^2\,h_0(v_\lambda)/z'(|v_\lambda|)^3]. \tag{3.73}$$

Writing in the form of $N_2(\lambda)$ from equation (3.49) we see that the expansion coefficients $b(\lambda)$ can be given as

$$b(\lambda) = \frac{1}{A_2(\lambda)^2\,N_3(\lambda)}\int_{-\infty}^{\infty}\mathrm{d}v\,\zeta_2(v)\,\phi_{\mathrm{od}}(v,\lambda), \tag{3.74}$$

with
$$N_3(\lambda) = g(\infty,\lambda)^{-1}\,[R(\infty,\lambda)^2+\pi^2 g(\infty,\lambda)^2]. \tag{3.75}$$

The normalization constant $A_2(\lambda)$ is of course immaterial in the calculation of the initial-value solution (3.1), for which we have now given a complete algorithm.

3.5. *The 'symbolic' eigenfunctions*

If we attempt to formalize the above by defining new eigenfunctions

$$\Phi_{\mathrm{od}}(v,\lambda) = N_3(\lambda)^{-\frac{1}{2}}\,h_0(v)\,[R(v,\lambda)-\alpha(v,\lambda)], \tag{3.76}$$

then, provided that the integral sign is taken to stand for the whole of the foregoing analysis, we can consider the set orthonormal and write

$$\text{‘}\int\mathrm{d}v\,\Phi_{\mathrm{od}}(v,\lambda)\,\Phi_{\mathrm{od}}(v,\lambda') = \delta(\lambda-\lambda').\text{’} \tag{3.77}$$

With the same proviso, the function $b(\lambda)$ can be written as though it were the 'formal' Fourier coefficient:

$$b(\lambda) = \int_{-\infty}^{\infty}\mathrm{d}v\,\zeta_2(v)\,\Phi_{\mathrm{od}}(v,\lambda). \tag{3.78}$$

The above is what Case has called the 'symbolic' orthogonality property of singular eigenfunctions (Case & Zweifel 1967, p. 69). The use of 'symbolic' expressions in equations is fraught with considerable dangers of misunderstanding, as a number of mistakes in the neutron transport literature testify (see especially Kuščer & McCormick (1965) for a critical discussion). Hangelbroek (1973) has also objected to their application on the grounds that such expressions would seem to imply an indefinable product of distributions. We shall avoid unqualified use of expressions such as (3.77) and (3.78) so far as possible.

4. Solution by Laplace transform

In the introduction we promised to work out the connection between the singular eigenfunction solutions just obtained and the results of applying the Laplace transform to the same transport equation. If these were simple alternatives, on the level of textbook solutions for non-singular problems, this would be a superfluous exercise. But in the present model it proves to be of considerable interest both theoretically and practically: it both explains the nature of the singular eigenfunctions and provides the neatest proof of their completeness; and it leads to what is probably the simplest computational algorithm for obtaining the initial-value solutions $p(v, \tau)$. Neither of these aspects can be said to be familiar: the pseudofunction $\mathrm{Pf}\,R(v, \lambda)$ seems virtually new to statistical mechanics, while the computational methods referred to, involving numerical inversion of the Laplace transform, are still little appreciated among physicists.†

4.1. *Transformation of the initial-value problem*

Although, as in the singular eigenfunction method, the problem may be split into treatments of odd and even parity components, this proves to be of little advantage and we can defer parity considerations until a later stage. We shall follow the approach given by Barker *et al.* (1977) with minor differences of scaling.

Let us begin by factoring out $h_0(v)$ so as to define

$$p(v, \tau) = h_0(v)\, F(v, \tau). \tag{4.1}$$

The transport equation (2.5) thus becomes

$$\frac{\partial F(v, \tau)}{\partial \tau} = \int_{-\infty}^{\infty} \mathrm{d}u\, |v-u|\, h_0(u)\, F(u, \tau) - z(v)\, F(v, \tau). \tag{4.2}$$

On applying the Laplace transform

$$f(v, s) = \int_0^{\infty} \mathrm{e}^{-s\tau}\, F(v, \tau)\, \mathrm{d}\tau \tag{4.3}$$

to the above, it follows that

$$[z(v) + s] f(v, s) = \int_{-\infty}^{\infty} \mathrm{d}u\, |v-u|\, h_0(u) f(u, s) + F(v, 0), \tag{4.4}$$

in which $F(v, 0) = p(v, 0)/h_0(v)$ gives the initial condition. Let it be emphasized once again that the present procedure makes no demands on the nature of $p(v, 0)$ other than that it should possess a Laplace transform. The class of acceptable initial conditions will certainly include all 'reasonable' probability distributions including the 'fundamental' condition: $p(v, 0) = \delta(v - v_0)$.

Unlike the eigenvalue equation of the previous section, equation (4.4) can be shown to be exactly soluble by essentially 'elementary' means. We first differentiate both sides twice with respect to v using the symbolic relation $(\mathrm{d}^2/\mathrm{d}v^2)|u-v| = 2\delta(u-v)$ and, after some rearrangement, find the differential equation

$$[z(v) + s] f''(v, s) + 2z'(v) f'(v, s) = F''(v, 0). \tag{4.5}$$

† In § 4.1 we retrace the method of Barker *et al.* (1977). An independent, but essentially similar, approach was used by the late Pierre Résibois who, in brilliant, if insouciant, manner, derived the results of Barker *et al.* without explicit reference either to the eigenvalue spectrum or the singular nature of the problem. Moreover his treatment of the spatially non-uniform transport problem, to which we turn in § 7, anticipates ours and is the first published solution for this form of the Rayleigh model (Résibois 1978). See also the footnote to § 5.3.

The left-hand side proves to have the integrating factor $z(v)+s$ and on using this we obtain a solution of (4.4) in the following indefinite integrals:

$$f(v,s)=\int^{v}\frac{\mathrm{d}u}{[z(u)+s]}\int^{u}\mathrm{d}w[z(w)+s]\,F''(w,0)+a(s)\int^{v}\frac{\mathrm{d}u}{[z(u)+s]^{2}}+b(s). \tag{4.6}$$

Here $a(s)$ and $b(s)$ are functions that account for the lost boundary conditions. Since F'' appears under the inner integral, we can integrate twice by parts and have various choices of how to rearrange the result. We adopt the following as easiest for division into parity components:

$$f(v,s)=\frac{p(v,0)}{h_0(v)\,[z(v)+s]}-2\int_{v}^{\infty}\frac{\mathrm{d}u}{[z(u)+s]^{2}}\int_{0}^{u}\mathrm{d}w\,p(w,0)+A(s)\int_{0}^{v}\frac{\mathrm{d}u}{[z(u)+s]^{2}}+B(s), \tag{4.7}$$

with $A(s)$, $B(s)$ still unknown. At this point there is a choice whether to substitute back into equation (4.2) and its once-differentiated counterpart, or to take advantage at once of the parity properties of the solution. Taking the latter course, we define components $f_{\mathrm{ev}}(v,s)$, $f_{\mathrm{od}}(v,s)$ in the usual way (cf. (2.20) and (2.21)) and, remembering that $z(v)$ is *even*, obtain the two equations

$$f_{\mathrm{ev}}(v,s)=\frac{p_{\mathrm{ev}}(v,0)}{h_0(v)\,[z(v)+s]}-2\int_{v}^{\infty}\frac{\mathrm{d}u}{[z(u)+s]^{2}}\int_{0}^{u}\mathrm{d}w\,p_{\mathrm{ev}}(w,0)+C(s), \tag{4.8}$$

$$f_{\mathrm{od}}(v,s)=\frac{p_{\mathrm{od}}(v,0)}{h_0(v)\,[z(v)+s]}-2\int_{0}^{v}\frac{\mathrm{d}u}{[z(u)+s]^{2}}\int_{u}^{\infty}\mathrm{d}w\,p_{\mathrm{od}}(w,0)+D(s)\int_{0}^{v}\frac{\mathrm{d}u}{[z(u)+s]^{2}}. \tag{4.9}$$

The functions $C(s)$ and $D(s)$ remain undetermined but can be found by substituting back into the parity-separated versions of (4.4). After lengthy integrations, requiring all the properties (2.35)–(2.38) of $z(v)$, we arrive at the expressions

$$C(s)=1/s \tag{4.10}$$

and

$$D(s)=\frac{1}{Y(v,s)}\int_{0}^{\infty}\mathrm{d}u\,p_{\mathrm{od}}(w,0)\,Y(u,s), \tag{4.11}$$

with $Y(v,s)$ defined by

$$Y(v,s)=\int_{0}^{v}\frac{\mathrm{d}u}{[z(u)+s]^{2}}. \tag{4.12}$$

The behaviour of the function $Y(v,s)$ will prove to be crucial to the explanation of the results.† In the solution so far it is clear that the function $C(s)$ dominates increasingly as $\tau\to\infty$ $(s\to 0)$ and provides the equilibrium distribution $h_0(v)$. The initial distribution is accounted for by the first terms, dominant for $s\to 0$, and the integrals represent the more or less complicated transient in the intermediate time-range.

When we consider the Laplace inversion of the above formulae, it is clear that three very different types of operation are involved. In the first the standard inversions $\mathscr{L}^{-1}\{s^{-1}\}$ and $\mathscr{L}^{-1}\{[z(x)+s]^{-2}\}$ give rise to the equilibrium distribution $h_0(v)$ and the exponential transient $p(v,0)\exp(-z(v)\,\tau)$ respectively. The second type of operation occurs in the terms that are a functional of the initial conditions. Here we need to take the operator $\mathscr{L}^{-1}$ under the integral

† While formally we can identify $Y(v,s)=R(v,-s)$, we are obliged to emphasize the role of Y as a function of the complex variable s by the change of notation. Looking forward to equation (7.21) we may also note the role of $Y(v,s)$ as the special case $Y(v,s)=U(0,v,s)$.

sign, a procedure which can be justified, but which requires care. Thirdly, there is the altogether more problematic operation

$$\mathscr{L}^{-1}\left[\frac{Y(v,s)}{Y(\infty,s)}\int_0^\infty \mathrm{d}u\, p(u,0)\, Y(u,s)\right], \tag{4.13}$$

in which, we may easily anticipate, the difficulties of the *odd* singular eigenfunctions reside.

If we tentatively assume the inversion of the 'distributed' Laplace transforms to be valid, i.e. that

$$\mathscr{L}^{-1}\left\{\int_0^v \frac{\mathrm{d}u}{[z(u)+s]^2}\right\} = \tau\int_0^v \mathrm{d}u \exp\left[-z(u)\,\tau\right], \tag{4.14}$$

we may collect the solution together in the form

$$\begin{aligned} p(v,\tau) &= \underset{\text{(mixed)}}{p(v,0)\,\mathrm{e}^{-z(v)\tau}} + \underset{\text{(even)}}{h_0(v)} \\ &\quad -2\tau h_0(v)\left[\underset{\text{(even)}}{\int_v^\infty \mathrm{d}u\, \mathrm{e}^{-z(u)\tau}\int_0^u \mathrm{d}w\, p_{\mathrm{ev}}(w,0)} + \underset{\text{(odd)}}{\int_0^v \mathrm{d}u\, \mathrm{e}^{-z(u)\tau}\int_u^\infty \mathrm{d}w\, p_{\mathrm{od}}(w,0)}\right] \\ &\quad + \mathscr{L}^{-1}\left[\underset{\text{(odd)}}{\frac{Y(v,s)}{Y(\infty,s)}\int_0^\infty \mathrm{d}u\, p_{\mathrm{od}}(u,0)\, Y(u,s)}\right] \end{aligned} \tag{4.15}$$

with the parities of the separate terms as marked.

The special case for $p(v,0) = \delta(v-v_0)$ is worth noting and, since the superposition principle holds, can be said to imply knowledge of the above. We find that

$$\begin{aligned} p(v,v_0,\tau) &= \underset{\text{(mixed)}}{\delta(v-v_0)\,\mathrm{e}^{-z(v_0)\tau}} + \underset{\text{(even)}}{h_0(v)} \\ &\quad -\tau h_0(v)\left[\underset{\text{(even)}}{\int_{\max(|v|,|v_0|)}^\infty \mathrm{d}y\, \mathrm{e}^{-z(y)\tau}} + \underset{\text{(odd)}}{\operatorname{sgn}(v)\operatorname{sgn}(v_0)\int_0^{\min(|v|,|v_0|)} \mathrm{d}y\, \mathrm{e}^{-z(y)\tau}}\right] \\ &\quad + \underset{\text{(odd)}}{h_0(v)\mathscr{L}^{-1}[B(v,v_0,s)]}, \end{aligned} \tag{4.16}$$

where
$$B(v,v_0,s) = Y(v,s)\,Y(v_0,s)/Y(\infty,s). \tag{4.17}$$

We shall see later that important results, for example the *velocity autocorrelation function* $S_v(\tau)$, can be obtained directly from the above equation without explicit evaluation of the inverse in the last term. First, however, we shall consider the Laplace inverses $\mathscr{L}^{-1}[Y(v,s)]$ and $\mathscr{L}^{-1}[B(v,v_0 s)]$ in detail. Although the solution of the first is 'elementary', it is not a pure formality and the intermediate stages in its proof are of direct importance to the second.

4.2. *Regular inverses*

Consider the Laplace inverse of the function $Y(v,s)$ defined in (4.12). The inversion integral reads

$$\mathscr{L}^{-1}[Y(v,s)] = \frac{1}{2\pi\mathrm{i}}\int_{\sigma-\mathrm{i}\infty}^{\sigma+\mathrm{i}\infty} \mathrm{d}s\, \mathrm{e}^{s\tau}\int_0^v \frac{\mathrm{d}y}{[z(y)+s]^2}, \tag{4.18}$$

with the contour to the right of all singularities. Given that $z(v) \geqslant 1$ in the scaled variable, it is clear that singularities are confined to the branch-cut running from $s = -1$ to $s = -z(v)$ on the negative real axis. The bound $1 \leqslant z(v) \leqslant 1+|v|$ ((2.40)) enables us to write

$$|Y(v,s)| \leqslant |v|/|s+1|^2, \tag{4.19}$$

while we note for later use that

$$|Y(v,s)| > \left|\int_0^\infty \frac{\mathrm{d}y}{(1+s+y)^2}\right| = \frac{1}{|s+1|}. \tag{4.20}$$

To find the required inverse we make up the closed contour shown in figure 5 and consider the contributions for each segment in the usual way. In the limit $R \to \infty$ the contributions from the segments marked Γ_R^+ and Γ_R^- vanish, likewise that from the small semicircle as $\epsilon \to 0$. The integral is therefore determined by the contributions from Γ_+ and Γ_- along the branch-cut, which we must now examine. Let $s = \lambda \pm i\epsilon$ be conjugate points across the cut and make the abbreviation

$$Y^{\pm}(\lambda) = \lim_{\epsilon\to\infty} Y(v, -\lambda \pm i\epsilon). \tag{4.21}$$

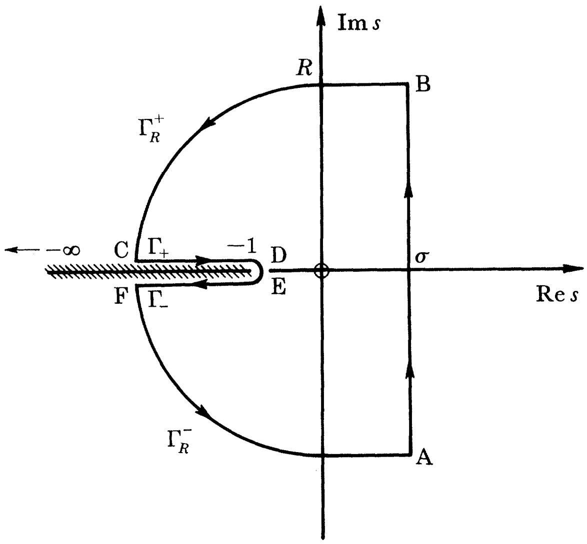

FIGURE 5. Contour for the evaluation of the inverse transformation $\mathscr{L}^{-1}[B(v, v_0, s)]$ of equations (4.17) and (4.28). The branch-cut extending to $-\infty$ is shown by the hatched line.

Then we can write the inverse

$$\mathscr{L}^{-1}[Y(v,s)] = \frac{1}{2\pi i}\int_1^{z(v)} d\lambda\, e^{-\lambda v}[Y^-(\lambda) - Y^+(\lambda)]. \tag{4.22}$$

On using the identity

$$\lim_{\epsilon\to 0}\frac{1}{[z(v)-\lambda \pm i\epsilon]^2} = \frac{\mathrm{Pf}}{[z(v)-\lambda]^2} \pm i\pi\,\delta'[z(v)-\lambda] \tag{4.23}$$

and its antiderivative

$$\lim_{\epsilon\to 0} Y(v, -\lambda \pm i\epsilon) = R(v,\lambda) \pm i\pi \int^v dy\,\delta'[z(y)-\lambda], \tag{4.24}$$

it is evident that the integral on the right is none other than the function $g(v,\lambda)$ defined in (3.66), which arose in the singular eigenfunction solution. Thus we can assert that

$$\left.\begin{aligned} Y^+(\lambda) &= R(v,\lambda) + i\pi\, g(v,\lambda), \\ Y^-(\lambda) &= R(v,\lambda) - i\pi\, g(v,\lambda) \end{aligned}\right\} \tag{4.25}$$

with $g(v,\lambda)$ the required combination of δ and H-functions (cf. 3.66). Using these we find that

$$\begin{aligned} \mathscr{L}^{-1}\{Y(v,s)\} &= -\int_0^{|v|} dv_\lambda\, e^{-z(v_\lambda)\tau} z(v_\lambda)\, g(v,\lambda) \\ &= -\int_0^{|v|} dv_\lambda \left[\frac{z''(v_\lambda)}{z'(v_\lambda)^2}\right] e^{-z(v_\lambda)\tau}[H(v-|v_\lambda|) - H(-v-|v_\lambda|)] \\ &\quad -\int_0^{|v|} dv_\lambda \frac{e^{-z(v_\lambda)\tau}}{z'(v_\lambda)}[\delta(v-|v_\lambda|) - \delta(v+|v_\lambda|)]. \end{aligned}$$

On using the fact that $z''(v_\lambda)/z'(v_\lambda)^2 = (\mathrm{d}/\mathrm{d}v_\lambda)\,(z'(v_\lambda)^{-1})$ and integrating the first term on the right by parts, we obtain a term exactly cancelling the second plus the expected transient term. In this way it emerges that

$$\mathscr{L}^{-1}[Y(v,s)] = \tau\int_0^v \mathrm{d}y\,\mathrm{e}^{-z(y)\tau}. \tag{4.26}$$

Reference back to (3.24) makes it clear that we can write

$$p_{\mathrm{ev}}(v,v_0,\tau) = h_0(v) + \int_1^\infty \mathrm{d}\lambda\,\mathrm{e}^{-\lambda\tau}\,\Phi_{\mathrm{ev}}(v_0,\lambda)\,\Phi_{\mathrm{ev}}(v,\lambda), \tag{4.27}$$

recognizing that the $\tau\to 0$ form of this is just the completeness relation for orthonormalized versions Φ_{ev} of the even eigenfunctions ϕ_{ev} of equation (3.24). (We need not, of course, characterize the above as 'formal' since there is no problem in inverting integrations.)

In this way we have both justified the taking of the Laplace transform inverse operator under the integral sign and exposed the essential connection between the eigenfunctions ϕ_{ev} and certain real integrals arising out of the *even* transform solution. We shall comment further on the importance of (4.24) and (4.25) after treating the *odd* solutions.

4.3. *Singular inverses*

We now consider the inverse

$$\mathscr{L}^{-1}[B(v,v_0,s)] = \frac{1}{2\pi\mathrm{i}}\int_{\sigma-\mathrm{i}\infty}^{\sigma+\mathrm{i}\infty}\mathrm{d}s\,\mathrm{e}^{s\tau}\left[\frac{Y(v_0,s)\,Y(v,s)}{Y(\infty,s)}\right]. \tag{4.28}$$

The function fails to be analytic along the whole of the negative real axis cut from $s=-1$ to $s=-\infty$, by virtue of the denominator $Y(\infty,s)$.† Moreover, the combination of the two bounds (4.19) and (4.20) shows that

$$|B(v,v_0,s)| \leqslant |v_0 v|/(1+|s+1|^3). \tag{4.29}$$

As before, we choose the contour shown in figure 5, noting that the above inequality guarantees the vanishing of contributions from the large arcs. Once again the only contribution is from the neighbourhoods of the branch-cut. This leads now to an infinite integral, and we find that

$$\mathscr{L}^{-1}[B(v,v_0,s)] = \frac{1}{2\pi\mathrm{i}}\int_1^\infty \mathrm{d}\lambda\,\mathrm{e}^{-\lambda\tau}[B^-(\lambda)-B^+(\lambda)], \tag{4.30}$$

where
$$B^{\pm}(\lambda) = \lim_{\epsilon\to 0} B(v,v_0,-\lambda\pm\mathrm{i}\epsilon). \tag{4.31}$$

Now the limit may easily be obtained in terms of the functions $R(v,\lambda)$ and $g(v,\lambda)$ by using the result (4.25). Reassuringly, it emerges that

$$\begin{aligned} B(v,v_0,-\lambda\pm\mathrm{i}\epsilon) &= \frac{Y(v,-\lambda\pm\mathrm{i}\epsilon)\,Y(v_0,-\lambda\pm\mathrm{i}\epsilon)}{Y(\infty,-\lambda\pm\mathrm{i}\epsilon)} \\ &= \frac{Y(v,-\lambda\pm\mathrm{i}\epsilon)\,Y(v_0,-\lambda\pm\mathrm{i}\epsilon)\,Y(\infty,-\lambda\pm\mathrm{i}\epsilon)}{R(\infty,\lambda)^2+\pi^2 g(\infty,\lambda)^2}, \end{aligned} \tag{4.32}$$

† The type of 'distributed' Laplace transform treated here is seldom considered even in otherwise comprehensive works. A rare exception is Churchill (1958).

with the inevitable resemblance to the normalization factor $N_3(\lambda)$ of equation (3.75). Applying (4.25) to the denominator we then find

$$\frac{B^-(\lambda)-B^+(\lambda)}{2\pi i}=\frac{g(\infty,\lambda)}{A(\lambda)}\left[R(v,\lambda)\,R(v_0,\lambda)-\pi^2 g(v_0,\lambda)\,g(v,\lambda)\right]$$
$$-\frac{R(\infty,\lambda)}{A(\lambda)}\left[R(v,\lambda)\,g(v_0,\lambda)+R(v_0,\lambda)\,g(v,\lambda)\right]. \tag{4.33}$$

Thus, by returning this expression to (4.30), it can be recognized that we have reduced the desired Laplace inverse to a real integral. Moreover it will be clear that the form of this integral is precisely that dictated by the *odd* singular eigenfunctions. To see this we take the 'formally orthonormal' set Φ_{od} and note that these are related to the B-function through

$$\Phi_{od}(v,\lambda)=\left[\frac{h_0(v)\,g(\infty,\lambda)}{A(\lambda)}\right]^{\frac{1}{2}}\left[\frac{R(v,\lambda)-R(\infty,\lambda)\,g(v,\lambda)}{g(\infty,\lambda)}\right], \tag{4.34}$$

whence
$$\frac{B^-(\lambda)-B^+(\lambda)}{2\pi i}=\frac{\Phi_{od}(v,\lambda)\,\Phi_{od}(v_0,\lambda)}{h_0(v)}-\frac{g(v_0,\lambda)\,g(v,\lambda)}{g(\infty,\lambda)}. \tag{4.35}$$

The inversion integral has now become

$$h_0(v)\mathscr{L}^{-1}[B(v,v_0,s)]=\int_0^1 d\lambda\,\Phi_{od}(v_0,\lambda)\,\Phi_{od}(v,\lambda)\,e^{-\lambda\tau}$$
$$-h_0(v)\int_0^\infty dv_\lambda\left[\frac{g(v_0,\lambda)\,g(v,\lambda)}{g(\infty,\lambda)}\right]z'(v_\lambda)\,e^{-z(v_\lambda)\tau},$$

and the second integral can be evaluated by parts. After sorting out the δ- and H-components of the g-functions, we find that

$$\int_0^\infty dv_\lambda\,z'(v_\lambda)\,e^{-z(v_\lambda)\tau}\left[\frac{g(v_0,\lambda)\,g(v,\lambda)}{g(\infty,\lambda)}\right]$$
$$=\frac{\delta_{od}(v,v_0)\,e^{-z(v_0)\tau}}{h_0(v)}-\operatorname{sgn}(v)\operatorname{sgn}(v_0)\,t\int_0^{\min(|v|,|v_0|)}dy\,e^{-z(y)\tau}. \tag{4.36}$$

Both these terms are destined to cancel on their substitution back into (4.16) so that we arrive at the now inevitable result

$$p_{od}(v,v_0,\tau)=\int_1^\infty d\lambda\,e^{-\lambda\tau}\,\Phi_{od}(v_0,\lambda)\,\Phi_{od}(v,\lambda). \tag{4.37}$$

If we combine this with (4.27) after letting τ tend to zero, we obtain the 'formal' completeness relation

$$\delta(v-v_0)=h_0(v)+\int_1^\infty d\lambda\,\Phi_{ev}(v_0,\lambda)\,\Phi_{ev}(v,\lambda)+\int_1^\infty d\lambda\,\Phi_{od}(v_0\lambda)\,\Phi_{od}(v,\lambda). \tag{4.38}$$

Here we should perhaps emphasize that there is nothing contradictory about the appearance of the regular term $h_0(v)$ on the right: a precisely similar term arises to cancel it when the integrals are interpreted, just as happens in the $\tau\to 0$ limit of the transform solution.

With this we have completed the proof of completeness of both *even* and *odd* singular eigenfunctions by a method that is both simpler than that used in § 3.4 and *constructive* in character. Of no less importance, however, is the recognition, through equations (4.22)–(4.25) and (4.30)–(4.34), that the singular eigenfunctions ϕ_{ev} and ϕ_{od} may both be represented by the discontinuity in an otherwise holomorphic function on crossing the cut real axis. This is precisely the operation used by Bremmerman & Durand to define a new 'analytic function' approach to distribution theory (Bremmerman & Durand 1961, Bremmerman 1965). It is a particularly satisfying result of the present study that we may not only recognize the simplicity of the Bremmerman–Durand approach, compared for example with that of Schwartz (1966), but are even, as it were, 'forced' to adopt it by the very nature of our model.

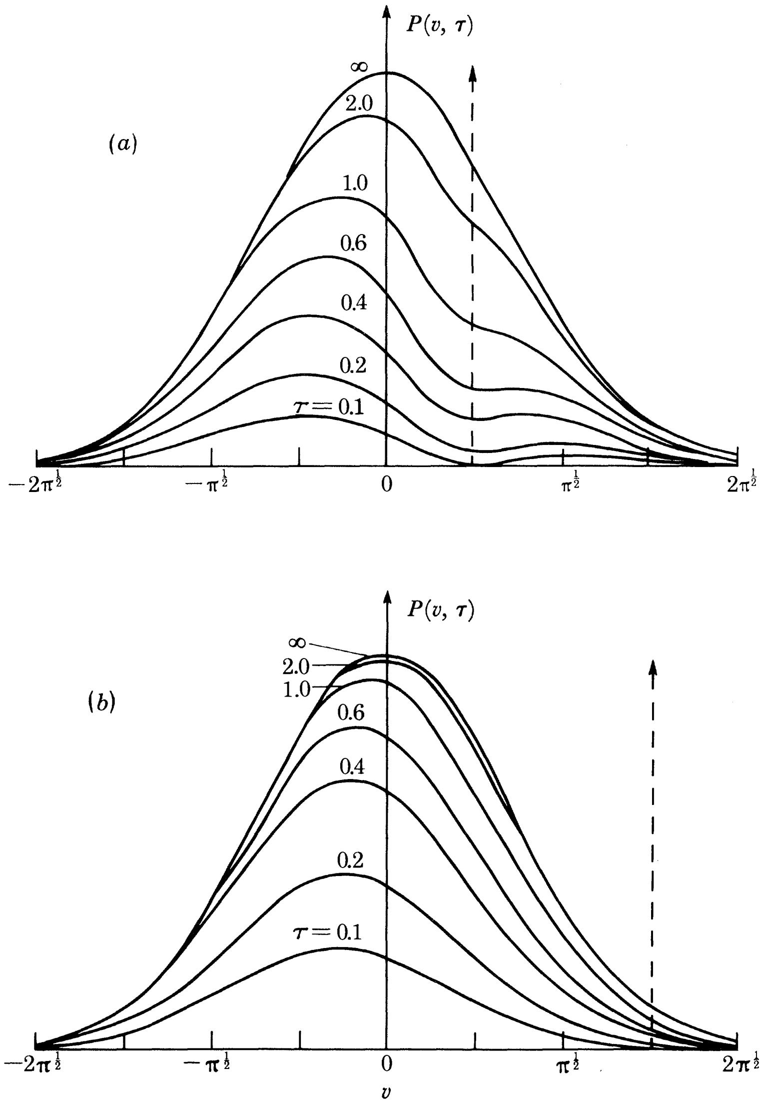

FIGURE 6. Relaxation of initial δ-functions in velocity (Maxwellian heat-bath). The initial conditions are (*a*) $P(v, 0) = \delta(v-0.5\pi^{\frac{1}{2}})$ and (*b*) $P(v, 0) = \delta(v-1.5\pi^{\frac{1}{2}})$. The curves describe $P(v, \tau)$ for the times τ as shown. The position of the initial δ-function is as indicated by dashed arrow, but its decay is not shown.

4.4. *Numerical Laplace inversions*

Our final observations in this section concern the use of numerical Laplace transform inversions to effect the computation of $p(v, \tau)$ from equations such as (4.15) and (4.16). Though the algorithms for numerical Laplace inversion are still little known, it is nowadays a relatively simple matter to compute functions such as $b(\tau) = \mathscr{L}^{-1}[B(s)]$ from the expression (4.17) and hence arrive at the full-range initial-value solution to almost any desired accuracy. The method of choice is the Dubner–Abate (D.–A.) procedure based on the alternative inversion integral

$$\mathscr{L}^{-1}[B(s)] = \frac{2e^{x\tau}}{\pi}\int_0^\infty dy\,\mathrm{Re}\,[B(s)]\cos y\tau \tag{4.39}$$

($s = x+iy$, $x > 0$; $\mathscr{L}^{-1}$ independent of x). This is first approximated by a Fourier series and then summed, with an optimal choice of x, by using complex FORTRAN for the extraction of the real parts.† Barker *et al.* (1977) computed the full-range relaxation of a δ initial distribution in a Rayleigh–Maxwellian heat-bath by this method with results reproduced here in figure 6. This is perhaps the first implementation of the D.–A. method for 'distributed' transforms and is an excellent example of its usefulness. While one might contemplate the numerical evaluation of the finite-part integrals involved in the singular eigenfunction method, it is doubtful whether this could easily match the simplicity of the Laplace transform procedure.

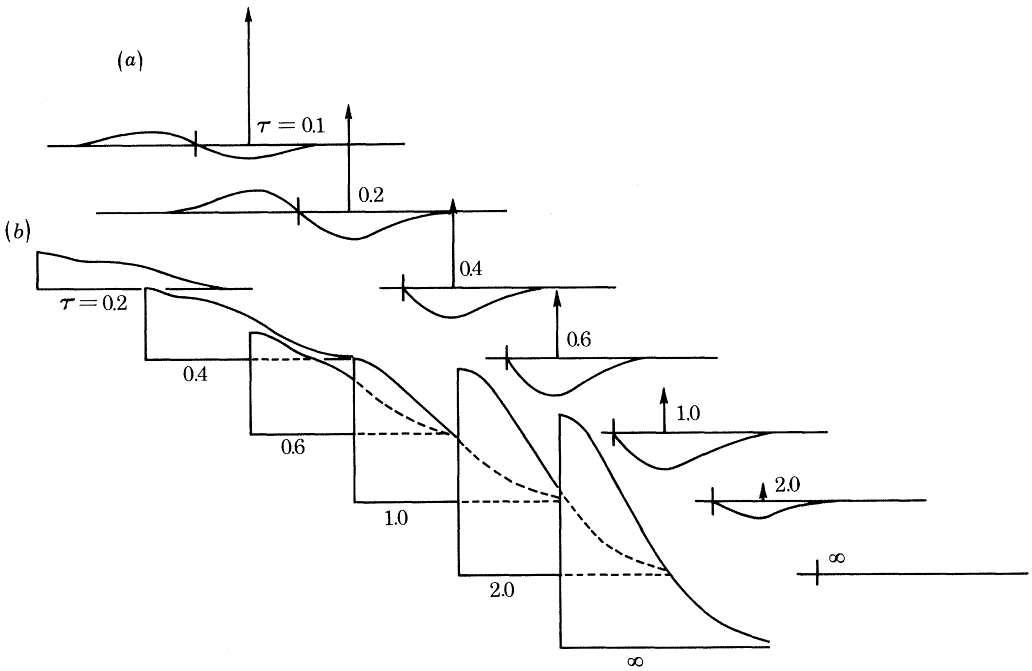

FIGURE 7. Separation of the parity components in velocity relaxation. (*a*) The *odd* component $P_{\mathrm{od}}(v, \tau)$ related to particle flux. (*b*) The *even* component $P_{\mathrm{ev}}(v, \tau)$ giving the speed relaxation. Both are for the initial condition $P(v, 0) = \delta(v-0.5\pi^{\frac{1}{2}})$ and the same time intervals as in figure 6. Only the positive half of most functions is shown, the negative part being the symmetrical or antisymmetrical continuation. The decay of the initial δ-function is here shown on a realistic scale.

The most general type of calculation we can do is that of the decay of an initial δ-distribution of velocity according to equation (4.16). The results for two different initial conditions are shown in figure 6, the curves shown representing the growth of the regular part of $p(v, \tau)$ at the given time intervals. The decay of the δ-function is not represented but can be inferred from the areas under the curves. Two qualitative effects are immediately apparent. First we see that there is no question of the δ-function 'spreading' about its base as would be natural in a diffusion-type

† In practice various improvements on the formula (4.39) are possible, which incorporate Im $[B(s)]$ as well as Re $[B(s)]$. We refer the reader to the original work of Dubner & Abate (1968) and to Durbin (1974) for further details.

process with predominantly local transitions. Next we note the marked asymmetry of the distribution $p(v,\tau)$ with the most probable velocity always in the *negative* direction when the singular component is excluded. This clearly reflects the anticorrelation of direction after one collision due to the enhanced probability of a 'head-on' first collision for those particles in the initial δ-distribution. The formation of a definite 'shoulder' on the positive side is presumably to be ascribed to the significant proportion of particles that collide twice during about one mean collision time. In figure 7 we have separated the two components $p_{\mathrm{ev}}(v,\tau)$ and $p_{\mathrm{od}}(v,\tau)$, each exhibited on the half-range. The main feature to be seen in the even component, corresponding to $p(|v|,\tau)$, is the relatively slow relaxation of particles having nearly zero velocity compared with that of particles in the high-velocity tails.

5. Moments and autocorrelation

As with any physical stochastic process, certain derived quantities, comprising less information than the full probability distribution function, are of considerable interest. Here we shall confine our attention to three of the most simple: the first moment of velocity, the first moment of speed and the velocity autocorrelation function.

5.1. *The mean velocity*

In forming the time-dependent first velocity moment, denoted $\langle v(\tau)\rangle$, we clearly need only consider the *odd* component of the distribution $p(v,\tau)$. Thus

$$\langle v(\tau)\rangle = \int_{-\infty}^{\infty} \mathrm{d}v\, v p(v,\tau) = 2\int_0^{\infty} \mathrm{d}v\, v p_{\mathrm{od}}(v,\tau). \tag{5.1}$$

If we now specialize to $p(v,0) = \delta(v-v_0)$, writing the mean as $\langle v(\tau)|v_0\rangle$, its time-dependence can be derived by direct integration of the solution (4.15) giving:

$$\langle v(\tau)|v_0\rangle = v_0\,\mathrm{e}^{-z(v_0)\tau} - 2\,\mathrm{sgn}\,(v_0)\,\tau\int_0^{\infty}\mathrm{d}v\, vh_0(v)\int_0^{\min(|v|,\,|v_0|)}\mathrm{d}u\,\mathrm{e}^{-z(u)\tau}$$
$$+2\mathscr{L}^{-1}\left[\frac{Y(x_0,s)}{Y(\infty,s)}\int_0^{\infty}\mathrm{d}v\,h_0(v)\,Y(v,s)\right]. \tag{5.2}$$

On using the identity $(\mathrm{d}/\mathrm{d}v)\,[vz'(v)-z(v)] = 2vh_0(v)$ and the integral

$$2\int_0^{\infty}\mathrm{d}v\, vh_0(v)\,Y(v,s) = 1-sY(\infty,s), \tag{5.3}$$

while noting that, by the derivative theorem of the Laplace transform,

$$sY(v,s) = \mathscr{L}\left\{\frac{\partial}{\partial\tau}\left[\tau\int_0^{v}\mathrm{d}y\,\mathrm{e}^{-z(y)\tau}\right]\right\},$$

we arrive at the simple result

$$\langle v(\tau)|v_0\rangle = \mathscr{L}^{-1}[Y(v_0,s)/Y(\infty,s)]. \tag{5.4}$$

It is easily confirmed that this contains the correct initial condition $\langle v(0)|v_0\rangle = v_0$ and implies the symmetric equilibrium $\langle v(\infty)|v_0\rangle = 0$. The principle of superposition converts all these results into equivalents for the evolution of a distributed initial state.

On applying the results of § 4 to the evaluation of the inverse, the above can be expressed equivalently in terms of integrals over the singular eigenfunctions. The final result is then

$$\langle v(\tau)\,|v_0\rangle = \int_0^\infty \mathrm{d}v_\lambda\, A(\lambda)^{-1}\, z'(v_\lambda)\, \mathrm{e}^{-z(v_\lambda)\tau}[R(v_0,\lambda)\, g(\infty,\lambda) - R(\infty,\lambda)\, g(v_0,\lambda)], \tag{5.5}$$

with $g(.,.)$ as always the function defined in (3.66). While this equation is explicit in time and mathematically more interesting, equation (5.4) is to be preferred for numerical calculations (see § 5.5).

5.2. *The mean speed*

As is to be expected, the determination of the *speed* relaxation is relatively simple since only the *even* solution is involved. The result follows directly from (4.15) after some obvious partial integrations. For the initial δ-distribution we find

$$\langle |v(\tau)|\; |v_0\rangle = \int_{|v_0|}^\infty \mathrm{d}y[(z(y)-1)\,\tau - 1]\,\mathrm{e}^{-z(y)\tau}, \tag{5.6}$$

other possibilities being represented as before by superposition. This equation brings out particularly clearly the complete lack of 'exponential' character in the solutions, whatever the time-régime.

5.3. *The velocity autocorrelation function*

The simplicity of the velocity autocorrelation function shows itself further in the autocorrelation function for equilibrium fluctuations. This we define as

$$\begin{aligned} S_v(\tau) &= \langle (v(0)\,|v_0)\;(v(\tau)\,|v_0)\rangle_{\mathrm{eq}} \\ &= 2\int_0^\infty \mathrm{d}v_0\, v_0\, h(v_0)\,\langle v(\tau)\,|v_0\rangle, \end{aligned} \tag{5.7}$$

the first expression indicating an average over the equilibrium ensemble. The function $S_v(\tau)$ is both an interesting characterization of the system in itself and the starting point for calculations of the response of a Rayleigh ensemble to external perturbations, such as an electric field.

Application of the transform solution (4.15) in the above integral gives

$$S_v(\tau) = 2\mathscr{L}^{-1}\left[\frac{1}{Y(\infty,s)}\int_0^\infty \mathrm{d}v_0\, v_0\, h_0(v)\; Y(v_0,s)\right],$$

which simplifies to

$$S_v(\tau) = \mathscr{L}^{-1}[Y(\infty,s)^{-1} - s]. \tag{5.8}$$

In spite of its appearance, this inverse is not in fact singular and can be used as a computational algorithm for $S_v(\tau)$. The corresponding expression in singular eigenfunctions is derivable as before with the result

$$S_v(\tau) = \int_0^\infty \frac{\mathrm{d}v_\lambda\, z'(v_\lambda)\, g(\infty,\lambda)\; e^{-z(v_\lambda)\tau}}{R(\infty,\lambda)^2 + \pi^2 g(\infty,\lambda)^2}. \tag{5.9}$$

The long-time asymptotic behaviour of the function $S_v(\tau)$ is of particular interest and its analysis provides a rare example of 'non-standard' Laplace transform theory. The essential problem is to find the corresponding behaviour of the function $Y(s,\infty)$ for $s \to 0$, which must dominate the inverse (5.8). Using the derivative theorem for the transform, we have first that

$$\begin{aligned} sY(\infty,s) &= \mathscr{L}\left\{\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{L}^{-1}[Y(\infty,s)]\right\} + \mathscr{L}^{-1}[Y(\infty,s)]_{\tau=0} \\ &\underset{s\to 0}{\sim} \mathscr{L}\left\{\frac{\mathrm{d}}{\mathrm{d}\tau}\left[\tau\int_0^\infty \mathrm{d}u\exp\left(-z(u)\,\tau\right)\right]\right\}, \end{aligned} \tag{5.10}$$

since the second term (equal to $\lim_{s\to\infty} sY(\infty, s)$) is negligible at long times. Now the integral can also be treated asymptotically by using the expansion (2.39) for $z(v)$. In this way

$$\int_0^\infty du \exp(-z(u)\tau) \underset{\tau\to\infty}{\sim} \int_0^\infty du \exp[(-1-h_0(0)\,u^2+O(u^4))\,\tau]$$
$$\underset{\tau\to\infty}{\sim} \tfrac{1}{2}[\pi/h_0(0)]^{\frac{1}{2}}\,\tau^{-\frac{1}{2}}\,e^{-\tau}.$$

Constructing the previous expression we then find that

$$sY(\infty, s) \underset{s\to 0}{\sim} \tfrac{1}{2}[\pi/h_0(0)]^{\frac{1}{2}}\mathscr{L}[\tau^{-\frac{1}{2}}(1-2\tau)\,e^{-\tau}].$$

Now the Laplace transform on the right exists and is equal to $\pi^{\frac{1}{2}}s(s+1)^{-\frac{3}{2}}$, so asymptotically

$$Y(\infty, s)^{-1} \underset{s\to 0}{\sim} (\tfrac{1}{2}\pi)\,h_0(0)^{\frac{1}{2}}\,(s+1)^{\frac{3}{2}}. \tag{5.11}$$

Returning to equation (5.8) we see that the asymptotic dependence in time is singular in precisely the sense of the formula

$$\mathscr{L}^{-1}(s^a) = \mathrm{Pf}[\tau^{-a-1}/\Gamma(-a)]\,H(\tau) \quad (a>0;\ a\neq 1, 2, \ldots)$$

(cf. Doetsch 1974, Appendix). Since the singularity at $\tau = 0$ is irrelevant for present purposes, we can assert the asymptotic relation

$$S_v(\tau) \underset{\tau\to\infty}{\sim} 4\pi^{-\frac{3}{2}}\,h_0(0)^{\frac{1}{2}}\,\tau^{-\frac{5}{2}}\,e^{-\tau}. \tag{5.12}$$

On consideration of the form of (5.12), it would seem that the nature of the heat-bath enters only through a constant factor, the asymptotic time-dependence $\tau^{-\frac{5}{2}}e^{-\tau}$ being a universal characteristic of all Rayleigh models.†

5.4. *Transport properties*

As we have already indicated, the study of equilibrium fluctuations can lead both to a useful characterization of the system free of initial conditions and to definite computations of transport properties. The route to the latter lies through the well known Kubo formulae of linear-response theory (Kubo 1958, 1965). We shall see that these formulae take on a particularly simple aspect when interpreted through the Laplace transform of the velocity autocorrelation function in the spirit of the present derivations.

5.4.1. *Self-diffusion*

The Kubo formula for this case relates the self-diffusion coefficient D_0 for a test-particle to its velocity autocorrelation by

$$D_0 = \int_0^\infty S_v(\tau)\,d\tau. \tag{5.13}$$

† Equation (5.8) was first given by Barker *et al.* (1977) and discovered independently by Résibois (1978). Note, however, the serious misprint in Résibois's equation (3.5) where s appears as 1. This makes the following equation (correctly equivalent to our (5.14)) incomprehensible and also tends to disguise the singular nature of the problem.

This invites use of the Laplace transform integral theorem

$$\int_0^\infty S_v(\tau)\,\mathrm{d}\tau = \mathscr{L}[F(\tau)]_{s=0}$$

by virtue of which

$$D_0 = Y(\infty,0)^{-1} = \left[\int_0^\infty \frac{\mathrm{d}y}{z(y)^2}\right]^{-1}. \tag{5.14}$$

The integral is rapidly convergent and can be evaluated numerically for the Maxwellian heat-bath with $z(v)$ given by equation (2.46). We shall collect all numerical results on transport properties together in § 5.5.

5.4.2. *Admittance and electrical conductivity*

One of the most engaging aspects of the Rayleigh model is the question of how an ensemble of charged test-particles responds to an alternating applied electric field. The answer is provided by the *generalized admittance* of the system, σ, which quantity is again available through a linear-response formula. After Kubo, we now have that

$$\sigma(\omega) = \frac{\sigma_0}{D_0}\int_0^\infty \mathrm{e}^{\mathrm{i}\omega\tau}\,S_v(\tau)\,\mathrm{d}\tau, \tag{5.15}$$

in which $S_v(\tau)$ is the dimensionless velocity autocorrelation function and D_0 the self-diffusion coefficient already introduced. The quantity σ_0 represents the d.c. conductivity, related to the unscaled diffusion constant D through the Stokes–Einstein relation $\sigma_0 = De^2/k_B T$. Knowledge of the admittance as a function of frequency provides (*a*) the net current flowing in the system (proportional to $|\sigma|$), (*b*) the rate of dissipation of electrical energy into the heat-bath (proportional to $\mathrm{Re}\,(\sigma)$) and (*c*) the phase-lag between current and field ($\arctan[\mathrm{Im}\,(\sigma)/\mathrm{Re}\,(\sigma)]$).

The Laplace transform solution again provides a direct route to these quantities. We have only to substitute $-\mathrm{i}\omega$ for s in equation (5.8) to obtain

$$\sigma(\omega) = \frac{\sigma_0}{D_0}\left[\frac{1}{Y(\infty,-\mathrm{i}\omega)}+\mathrm{i}\omega\right]. \tag{5.16}$$

Writing the real and imaginary parts explicitly we find

$$\mathrm{Re}\,[\sigma(\omega)] = \frac{\sigma_0}{D_0\,|Y(\infty,-\mathrm{i}\omega)|^2}\int_0^\infty \mathrm{d}u\,\frac{z(u)-\omega^2}{[z(u)^2+\omega^2]^2}, \tag{5.17}$$

and

$$\mathrm{Im}\,[\sigma(\omega)] = \frac{\sigma_0}{D_0\,|Y(\infty,-\mathrm{i}\omega)|^2}\left[1-2\int_0^\infty \frac{z(u)\,\mathrm{d}u}{z(u)^2+\omega^2}\right]. \tag{5.18}$$

From these equations we see that the frequency responses of both $|\sigma|$ and $\mathrm{Re}\,\sigma$ show a broad decay from the maximum, d.c., value to zero at high frequencies, there being no possible tendency to resonance. Numerical values presented in the next section illustrate these aspects in detail.

5.5. *Numerical computations*

The numerical methods described in § 4.4 provide excellent means of calculating all the quantities expressed as inversions of a Laplace transform. Again we work directly with equations (5.4), (5.8) and (5.16) using complex FORTRAN for the integrals and extracting real and variable-imaginary parts as required. We shall only be able to present a selection of the many possible

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results here. All calculations refer to the Maxwellian heat-bath described in § 2.4 and we caution the reader again that the scaled velocity, v, used here differs from the velocity x used in Hoare & Rahman (1973), Barker *et al.* (1977) and Raval (1978) by the factor $\pi^{\frac{1}{2}}$.

5.5.1. *Autocorrelation functions*

In analysing the autocorrelation of equilibrium fluctuations, one of the main questions of interest is the extent to which the function $S_v(\tau)$ deviates from a pure exponential decay. While, for the Rayleigh model, equation (5.9) shows that there can be no question of a single exponential transient, we cannot immediately rule out the possibility that the distributed transient appearing there might prove to be close to an effective exponential at least in some important time-régime. The question is of more than passing interest in that conjectures have been made in the literature to the effect that *all* Markovian kinetic processes may be well approximated by a pure exponential autocorrelation $S_v^0(\tau)$ fixed by the initial slope of the actual function $[\partial S_v(\tau)/\partial\tau]_{\tau=0}$ (Cukier & Hynes 1976).

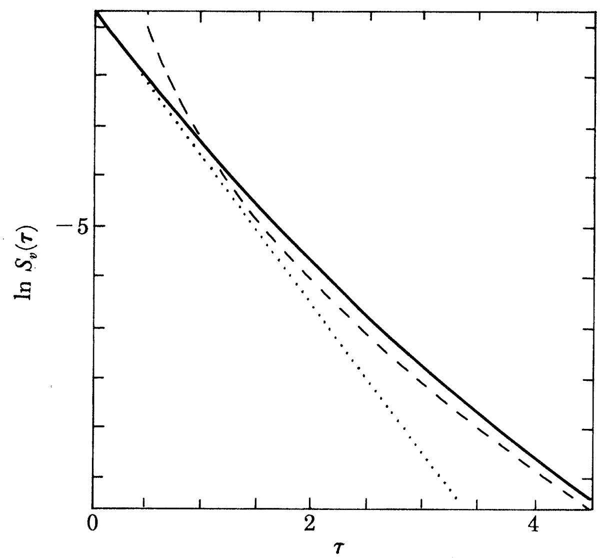

FIGURE 8. The velocity autocorrelation function for equilibrium fluctuations in an ensemble of Rayleigh test-particles (Maxwellian heat-bath). The solid line gives the value obtained by numerical inversion of the expression in equation (5.8); the dashed curve is the asymptotic approximation of equation (5.12); the dotted curve results from the estimate $S_v(\tau) = S_v(0)\exp\{-[\partial S_v(\tau)/\partial\tau]_{\tau=0}\tau\}$ (Cukier & Hynes 1976).

Figure 8 shows the decay of the velocity autocorrelation function of equilibrium fluctuations for a Rayleigh test-particle in a Maxwellian heat-bath, calculated by numerical inversion of the transform (5.8). The compensation of singular terms in the inversion integral of the D.–A. method was found to give no problems. The solid line representing the logarithm of the true function $S_v(\tau)$ may be compared with the dashed line representing the asymptotic result (5.12) and the dotted line resulting from the estimate $S_v(\tau) = S_v(0)\exp\{-[\partial S_v(\tau)/\partial\tau]_{\tau=0}\tau\}$ according to Cukier & Hynes. It is clear that the decay is significantly non-exponential at all times, as would be expected from the character of the spectrum, though perhaps rather less so than if the continuum were to fill the whole interval $\lambda \in (0, \infty)$ rather than $(1, \infty)$. The asymptotic result is remarkably good for all times appreciably greater than one mean collision-time.

5.5.2. *The diffusion coefficient*

An evaluation of the integral (5.14) with $z(x)$ for the Maxwellian heat-bath (2.46) leads to the result $D_0 = 1.031053\ldots$ in the present scaling. Reverting to unscaled units we find this equivalent to

$$D = 1.82749\ldots(na)^{-1}\,(2k_B\,T/\pi m)^{\frac{1}{2}},$$

the algebraic factor being the mean-free-path approximation to D in one dimension (n is the number density of particles, a the particle cross section). The excess over the mean-free-path value is not surprising and presumably reflects the predominant contribution from fast particles in the ensemble.

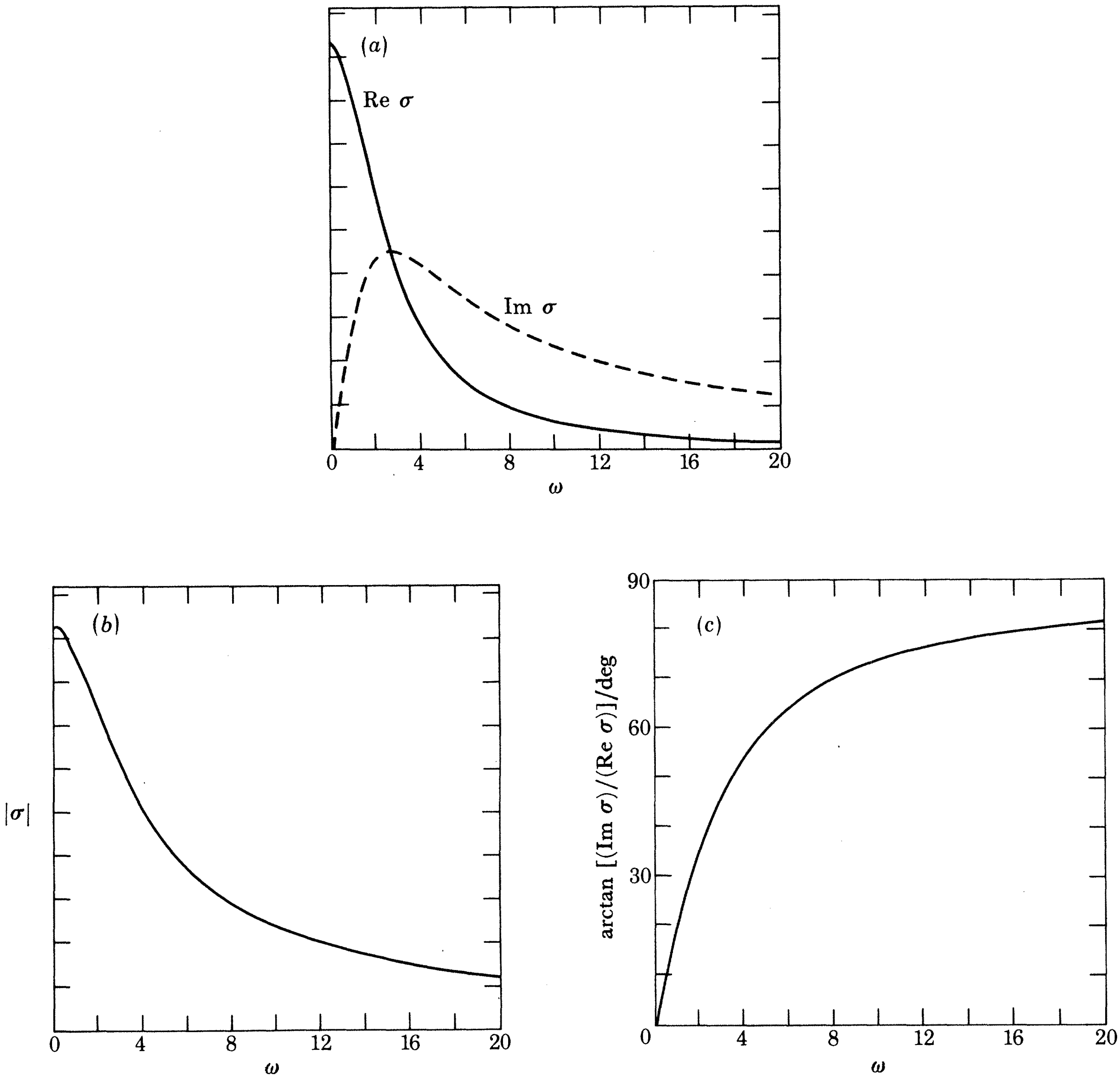

FIGURE 9. (*a*) Frequency dependence of the real and imaginary parts of the admittance, σ, for charged Rayleigh test-particles in a Maxwellian heat-bath. (*b*) Current in a charged Rayleigh test-particle ensemble as a function of applied frequency. (*c*) The phase-lag arctan$[(\mathrm{Re}\,\sigma)/(\mathrm{Im}\,\sigma)]$ under the same conditions. The ordinates in (*a*) and (*b*) are in arbitrary units.

5.5.3. *Electrical properties*

Values of the complex admittance $\sigma(\omega)$ were computed directly from equation (5.16) by using a complex FORTRAN quadrature for the integral $Y(\infty, -\mathrm{i}\omega)$. The values of $\mathrm{Re}[\sigma(\omega)]$, $\mathrm{Im}[\sigma(\omega)]$ and $|\sigma(\omega)|$ could then be tabulated as required.

The results, shown here in figures 9*a–c* correspond broadly to physical intuition. Thus, as to be expected, the dissipative component $\mathrm{Re}[\sigma(\omega)]$ is a maximum under d.c. conditions, falling with a bell-shaped decay to zero at high frequencies, though frequencies well in excess of the value $z^{-1}(0)$ are required effectively to suppress all energy-transfer from the field. Similarly, the current $|\sigma(\omega)|$ decreases with frequency, though with a less rapid approach to zero. At the same time the phase of current with respect to applied field lags systematically, the phase-angle increasing regularly from zero to $\frac{1}{2}\pi$ at infinite frequency. No vestige of resonance is seen.

6. Passage-time problems

An interesting, though little considered, aspect of the Rayleigh model is the computation of passage-time statistics in the presence of an absorbing barrier in the particle speed. Both upper and lower barriers can be considered, the former corresponding to the removal of fast particles at a hypothetical *activation energy* $E^{\dagger}$ for some chemical reaction, the latter to their removal at some lower threshold $E_{\dagger}$, perhaps also by chemical means. In fact both types of process are known in real systems of interest in 'hot-atom chemistry' (see for example Shizgal & Karplus 1971).

Although absorbing-barrier problems have been of interest for some time in physical chemistry (Montroll & Shuler 1958, Hoare 1964), most attention has been paid to the upper-barrier problem for internal degrees of freedom, such as vibration in molecules, and very little is known about systems without constant collision number, that is those with singular scattering kernels. The Rayleigh model appears to be the first known example of a singular Markovian model that is susceptible to a full passage-time analysis and we shall therefore examine it in detail, considering both upper and lower barriers. The most useful tool for this purpose will again be the Laplace transform method, but in using this we shall also be able to perceive the way in which the spectrum of the transition operator is modified by introduction of the barrier.

If we remember the equivalence between $2p_{\mathrm{ev}}(v,\tau)$ (half-range) and $p(|v|,\tau)$ (full-range), we may concentrate on determining the former in a manner which, up to the fitting of boundary conditions, is broadly parallel to the ordinary initial-value solution described in § 4.1. For brevity let the even components of the modified transport equations be written

$$\frac{\partial p_{\mathrm{ev}}(v,\tau)}{\partial\tau} = 2h_0(v)\left[\int_0^{v^{\dagger}} \mathrm{OR} \int_v^{\infty} \mathrm{d}u\right] \max(u,v)\, p_{\mathrm{ev}}(u,\tau) - z(v)\, p_{\mathrm{ev}}(v,\tau) \tag{6.1}$$

and their Laplace-transformed versions as

$$[z(v)+s] f_{\mathrm{ev}}(v,s) = 2\left[\int_0^{v^{\dagger}} \mathrm{OR} \int_{v_{\dagger}}^{\infty} \mathrm{d}u\right] \max(u,v)\, h_0(u) f_{\mathrm{ev}}(u,s) + F_{\mathrm{ev}}(v,0). \tag{6.2}$$

Here we have put $p_{\mathrm{ev}}(v,\tau) = h_0(v)\, F_{\mathrm{ev}}(v,\tau)$ and $f_{\mathrm{ev}}(v,s) = \mathscr{L}[F_{\mathrm{ev}}(v,\tau)]$ as in (4.1) and (4.3). We may now recognize that both alternatives correspond to the same differential equation (4.5) and that solutions similar to (4.8) may be constructed to satisfy the respective boundary conditions $f_{\mathrm{ev}}(v^{\dagger},\tau) = 0$ and $f_{\mathrm{ev}}(v_{\dagger},\tau) = 0$. The two types of barrier will now be considered separately.

6.1. *The upper absorbing barrier*

Specifying the upper-barrier solution as $f_{\mathrm{ev}}(v, v^\dagger, \tau)$, we see that equation (4.8) is modified to

$$f_{\mathrm{ev}}(v, v^\dagger, s) = \frac{p_{\mathrm{ev}}(v, 0)}{h_0(v)[z(v)+s]} - 2\int_v^{v^\dagger} \frac{\mathrm{d}u}{[z(u)+s]^2}\int_0^u \mathrm{d}w\, p_{\mathrm{ev}}(w, 0) + C(s, v^\dagger), \tag{6.3}$$

with the function $C(s, v^\dagger)$ to be determined by substitution back into the integral equation (6.2). Carrying out this process, with the use of the previously introduced partial integration formulae and properties of $z(v)$, we arrive at the result

$$C(s, v^\dagger) = \frac{1}{z'(v^\dagger)}\left[\frac{1}{z(v^\dagger)+s-v^\dagger z'(v^\dagger)} - \frac{1}{z(v^\dagger)+s}\right], \tag{6.4}$$

indicating the occurrence of two distinct exponential transients. The inversion of the transform is straightforward and we arrive at the explicit solution

$$p(|v|, v^\dagger, \tau) = p(|v|, v^\dagger, 0)\,\mathrm{e}^{-z(v)\tau} + \frac{2h_0(v)}{z'(v^\dagger)}[\![\exp\{[-z(v^\dagger)-v^\dagger z'(v^\dagger)]\,\tau\} - \exp[-z(v^\dagger)\,\tau]]\!]$$
$$-2\tau\, h_0(v)\int_v^{v^\dagger}\mathrm{d}u\,\mathrm{e}^{-z(u)\tau}\int_0^u \mathrm{d}w\, p(|w|, v^\dagger, 0) \quad (|v| < v^\dagger). \tag{6.5}$$

To obtain the response to an initial δ-distribution, we have only to write $\delta(v-v_0)\exp[-z(v_0)\,\tau]$ for the first term and in the last write a single integral with lower limit max $(|v|, |v_0|)$. Thus we have a solution which can accommodate regular and singular initial conditions equally well, including the rather natural case of an initially 'cold' ensemble: $p(|v|, v^\dagger, 0) = \delta(v)$.

An interesting feature of the above is the privileged position of the Maxwellian heat-bath distribution. Recalling the relation (2.47) which holds only for the Maxwellian, we see that the second term simplifies such that, in the present scaling,

$$p(|v|, v^\dagger, \tau) = p(|v|, v^\dagger, 0)\,\mathrm{e}^{-z(v)\tau} + \frac{2\mathrm{e}^{-v^2/\pi}}{\pi z'(v^\dagger)}[\exp(-\tau\pi^{-1}\,\mathrm{e}^{-v^{\dagger 2}/\pi}) - \mathrm{e}^{-z(v^\dagger)\tau}]$$
$$-\frac{2\tau\,\mathrm{e}^{-v^2/\pi}}{\pi}\int_v^{v^\dagger}\mathrm{d}u\,\mathrm{e}^{-z(u)\tau}\int_0^u \mathrm{d}w\, p(|w|, v^\dagger, 0). \tag{6.6}$$

This equation, in the alternative scaling, was first derived by Hoare & Rahman (1976).

One further special case is worth mention. If we take the initial condition

$$p(|v|, v^\dagger, 0) = 2h_0(v)/z'(v^\dagger); \quad 0 \leqslant v \leqslant v^\dagger,$$
$$= 0; \quad v^\dagger < v, \tag{6.7}$$

which (N.B. (2.35)) is an equilibrium distribution rescaled to the interval $(0, v^\dagger)$, we find, after a number of cancellations, the very simple result

$$p(|v|, v^\dagger, \tau) = [2h_0(v)/z'(v^\dagger)]\exp[-(z(v^\dagger)-v^\dagger z'(v^\dagger)\,\tau)]. \tag{6.8}$$

The meaning of this is that, if we take an equilibrium distribution and suddenly 'switch on' the absorbing barrier at $\tau = 0$, then the subsequent relaxation maintains the shape of the heat-bath distribution as it decays with rate-constant

$$\lambda_0(v^\dagger) = z(v^\dagger) - v^\dagger z'(v^\dagger). \tag{6.9}$$

As to be expected, $\lambda_0(v^\dagger) \to 0$ as $v^\dagger \to \infty$ and the effect of the barrier is nullified (N.B. (2.38)).

The above property is related to some further results of surprising simplicity. Let $C(\tau)$ represent the proportion of *un*reacted particles, those that have not passed the barrier at time τ. Then, on integrating the solution (6.5), we find, after various cancellations, that

$$C(\tau) = \int_0^{v^\dagger} p(v, v^\dagger, \tau) = \exp[-\lambda_0(v^\dagger)\,\tau], \tag{6.10}$$

with $\lambda_0(v^\dagger)$ as before. At the same time the distribution function for passage-times to the barrier is evidently

$$w_1(\tau) = -[\mathrm{d}C(\tau)/\mathrm{d}\tau] = \lambda_0(v^\dagger)\exp[-\lambda_0(v^\dagger)\tau], \tag{6.11}$$

and its first moment the *mean first-passage time* to reaction is

$$\langle\tau_1\rangle = \int_0^\infty \tau\, w_1(\tau)\,\mathrm{d}\tau = \int_0^\infty C(\tau)\,\mathrm{d}\tau = [\lambda_0(v^\dagger)]^{-1}. \tag{6.12}$$

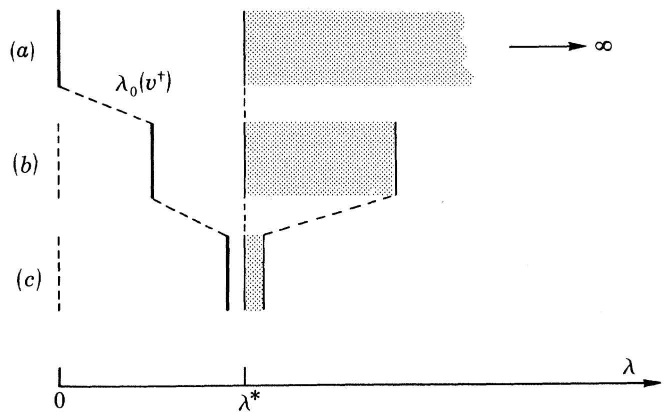

FIGURE 10. Eigenvalue spectra in relation to barrier height for the Rayleigh scattering operator truncated at an upper velocity absorbing barrier $v^\dagger$. (*a*) Spectrum for unperturbed relaxation ($v^\dagger \to \infty$). (*b*) Intermediate case. (*c*) Spectrum for the limiting régime $v^\dagger \ll 1$. The value of $\lambda_0(v\dagger)$ is given by equation (6.9).

In all the above the further simplification $\lambda_0(v^\dagger) = h_0(v^\dagger) = \pi^{-1}\exp(-v^{\dagger 2}/\pi)$ applies when the heat-bath distribution is Maxwellian. If we now define an *activation energy* $\epsilon^\dagger = v^{\dagger 2}/\pi$ in scaled units, it is clear that the above result is an 'Arrhenius Law' for the energy dependence of a first-order rate-constant. To put this into more familiar form, we return to the unscaled variables (equation (2.41) *et seq.*), define $E^\dagger = \frac{1}{2}MV^{\dagger 2}$, and obtain

$$\lambda_0(E^\dagger) = A\exp[-(E^\dagger/k_B T)], \tag{6.13}$$

with T the heat-bath temperature, and A dependent on the time-scaling.

Finally we return briefly to the relation between these results and the effect of the absorbing barrier on the spectrum of the transition operator. If we repeat the argument set out in § 3.1, this time with the barrier introducing an upper limit in the integral operator, we arrive at a condition involving the integral $R(v^\dagger, \lambda)$ instead of $R(\infty, \lambda)$. This can only be satisfied by the single discrete eigenvalue $\lambda_0(v^\dagger)$ in precisely the form (6.9). At the same time there must be an upper limit to the continuous spectrum imposed by the condition $z(v^\dagger) = \lambda^\dagger$, since no transients faster than this can contribute. The net effect is thus that, as $v^{\dagger} \to 0$, the single discrete eigenvalue encroaches on the point $\lambda^* = z(0)$ while the whole of the continuum is compressed towards the same from the other side. In the extreme case the system shows only the single transient $\exp(-\lambda^*\tau)$ since only those test-particles with effectively zero velocity survive beyond $\tau = 0$ to contribute. This process is illustrated schematically in figure 10.

A computation of the evolution of various initial δ-distributions in the presence of an upper barrier with the use of the solution (6.5) is illustrated in figure 11.

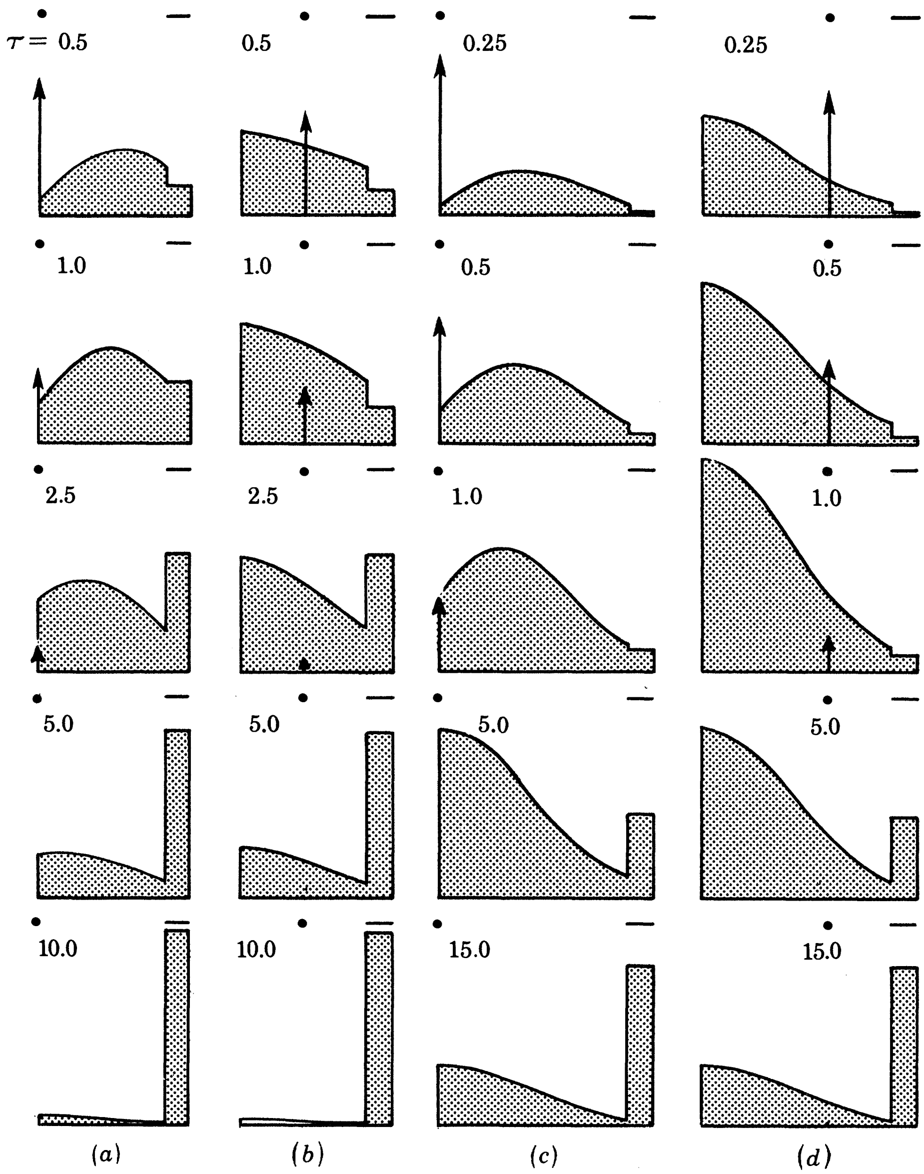

FIGURE 11. Relaxation of four different δ-ensembles of Rayleigh test-particles in the presence of an upper velocity-absorbing barrier and Maxwellian heat-bath. The vertical arrows represent the probability mass remaining in the δ-function, scaled to unity by the dot. The column on the right gives the integrated flux over the barrier scaled to unity by the horizontal bar. The figures give the elapsed time in reduced units. The positions of the initial δ-function, v_0, and the barrier height, $v^{\dagger}$, for the four cases are: (*a*) $v_0 = 0.0$, $v^{\dagger} = \pi^{\frac{1}{2}}$; (*b*) $v_0 = 0.5\pi^{\frac{1}{2}}$, $v^{\dagger} = \pi^{\frac{1}{2}}$; (*c*) $v_0 = 0.0$, $v^{\dagger} = 1.5\pi^{\frac{1}{2}}$; (*d*) $v_0 = 1.0\pi^{\frac{1}{2}}$, $v^{\dagger} = 1.5\pi^{\frac{1}{2}}$. Results were computed from equation (6.5).

6.2. *The lower absorbing barrier*

Although not obviously so at first sight, the lower-barrier problem proves to be considerably more complicated than the upper-barrier case. The difficulty lies in the nature of the boundary conditions, which now require vanishing of the solution as $v \to v_\dagger$ from above, the function $p(|v|, v_\dagger, \tau)$ being now interpreted on the infinite range $v \in (v_\dagger, \infty)$. To keep the manipulations under control we shall this time consider the δ-function initial condition from the outset. On examining equation (4.6) simplified in this way, it becomes clear that the only adequate solution must take the form

$$f(v,s) = \frac{\delta(v-v_0)}{h_0(v)\,[z(v)+s]} + \int_{v_\dagger}^{\max(v,v_0)} \frac{\mathrm{d}u}{[z(u)+s]^2} + C'(s,v_\dagger) + D'(s,v_\dagger)\int_{v_\dagger}^{v} \frac{\mathrm{d}u}{[z(u)+s]^2}, \qquad (6.14)$$

and that this will contain mixed odd and even components. Because of the two undetermined functions $C'(s, v_\dagger)$ and $D'(s, v_\dagger)$ we must substitute back into both the integral equation (6.2) and its once-differentiated form. After considerable work, we find these functions to be given by

$$D'(s,v_\dagger) = \frac{z'(v_\dagger)\,[z(v_\dagger)+s]\,[sR(v_0,\infty,s)-1]}{\{z'(v_\dagger)\,[z(v_\dagger)+s]\,[1-sR(v_\dagger,\infty,s)]+s\}} \qquad (6.15)$$

and

$$C'(s,v_\dagger) = 1/s[1-s\,R(v_\dagger,\infty,s)]\,[1+D'(s,v_\dagger)], \qquad (6.16)$$

with $R(a,b,s)$ a modified form of the previous R-integral defined as

$$R(a,b,s) = \int_a^b \frac{\mathrm{d}y}{[z(y)+s]^2}. \qquad (6.17)$$

The required solution then takes the form

$$p(|v|, v_\dagger, \tau) = p(|v|, v_\dagger, 0)\,\mathrm{e}^{-z(v_0)\tau} + \tau \int_{v_\dagger}^{\max(v,v_0)} \mathrm{d}u\,\mathrm{e}^{-z(u)\tau}$$
$$+\mathscr{L}^{-1}[C'(s,v_\dagger)] + \mathscr{L}^{-1}[D'(s,v_\dagger)\,R(v_\dagger,v,s)].$$

No further progress in reducing the two inverses analytically seems possible. They must therefore be treated numerically and the solutions for the initial δ-distribution superposed if distributed initial conditions apply. In spite of the complicated appearance of the results, it may be verified that the even component of equation (4.16) is correctly recovered in the limit $v_\dagger \to 0$. As may be suspected, the increased complexity found in the lower-barrier problem reflects the dominant contribution of the continuum eigenfunctions of both odd and even types. In fact it may be shown that the single discrete eigenvalue $\lambda_0(v^\dagger)$ present in the upper-barrier problem is absent when the lower barrier introduced.

7. The spatial transport problem

In the remaining sections of this paper we shall address the more demanding problem of the spatially inhomogeneous Rayleigh model, in which particle density itself evolves in time along with the velocity distribution. Various versions of this problem have been treated in the literature, notably by Nelkin & Ghatak (1964), Rahman *et al.* (1962) and, more recently, Résibois (1978). The problem is, of course, a long-standing aspect of neutron transport theory (see, for example, Williams 1966, 1971; Corngold 1964), though authors writing from the standpoint of 'kinetic theory' and the linearized Boltzmann equation have consistently failed to recognize this.

Nevertheless Résibois (1978), in a somewhat cryptic paper published just before his death, has left us with what amounts to a complete solution of the spatially inhomogeneous special Rayleigh problem. In this study some of the conclusions of Barker *et al.* (1977) and Raval (1978) are arrived at independently, though the latter's results are significantly extended by the removal of restrictions on the initial condition. The Résibois approach is, however, at some distance from the concerns of particle transport theory, makes no explicit reference to the singular nature of the scattering operator and its eigenvalue problem, and leaves a number of interesting particulars unexamined. We shall therefore derive a more explicit form of the solution in the present context while relating it to the earlier work cited and using the exact results now available to check the various approximations suggested there.

Our main object of interest is now the spatial–velocity distribution function $p(x, v, \tau)$ in which the scaling of distance $x \in (-\infty, +\infty)$ is taken to be that set out in § 2, namely $x = [Z(0)/V_0]\, X$ with $Z(0)$ the true collision frequency for stationary test-particles and V_0 the true mean speed for the heat-bath. Two types of normalization may be applied. Either (*a*) we assume p to be distributed over all space in the sense that

$$\int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}v\, p(x, v, \tau) = 1, \quad \text{for all} \quad \tau \tag{7.1}$$

or (*b*) we take periodic boundary conditions such that

$$\int_{x}^{x+l} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}v\, p(x, v, \tau) = 1, \quad \text{for all} \quad \tau \tag{7.2}$$

with the implication that $p(x, v, \tau) = p(x+l, v, \tau)$. In the former case it is appropriate to study the decay of a given initial distribution to an infinitely sparse state as $\tau \to \infty$; in the latter we study the approach to spatial homogeneity at given linear density. However, only alternative (*a*) will be taken up here.

The most general initial-value problem in these terms is where, at zero time, $p(x, v, 0)$ is an arbitrary bivariate distribution in position and velocity of the test-particles. However, a variety of special initial conditions are possible, several of which are of particular interest. We note the cases:

$$p(x, v, 0) = \rho(x)\, p(v, 0) \tag{7.3}$$

(positions and velocities initially uncorrelated),

$$p(x, v, 0) = \delta(x)\, p(v, 0) \tag{7.4}$$

(particles released at the origin with distributed velocities),

$$p(x, v, 0) = \rho(x)\, \delta(v - v_0) \tag{7.5}$$

(particles with identical velocity and distributed positions),

$$p(x, v, 0) = \rho(x)\, h_0(v) \tag{7.6}$$

(particles with equilibrated velocity and distributed positions),

$$p(x, v, 0) = \delta(x)\, h_0(v) \tag{7.7}$$

(particles released at origin with equilibrated velocity),

$$p(x, v, 0) = \delta(x)\, \delta(v - v_0) \tag{7.8}$$

(particles released at origin with identical velocities). Still other variations are possible if we specify the parity of the initial spatial or velocity distributions or both. Since, however, the system remains linear, the superposition principle allows us to work with the 'fundamental' solution, corresponding to (7.8), and construct all other cases from this if we wish.

While the eigenfunction approach to the problem is possible, and has figured prominently in neutron transport theory, the difficulties arising are enormously compounded on passing from the uniform to the spatially inhomogeneous case. We have, in fact, little choice but to stay within the framework of transform methods, and this we shall do apart from some general concluding remarks. Our approach will be to assume completely general initial conditions $p(x, v, \tau)$ throughout, avoiding the restriction to δ-functions (as in Résibois 1978) or initially equilibrated velocities (as in Raval 1978). These and other particular cases will then be considered by specialization of the main result.

7.1. *Solution of the general space- and time-dependent problem*

Our starting point is the full transport equation (2.4) with the Rayleigh kernel, namely

$$\left[\frac{\partial}{\partial\tau}+v\frac{\partial}{\partial x}+z(v)\right]p(x,v,\tau) = h_0(v)\int_{-\infty}^{\infty} du\,|v-u|\,p(x,u,\tau). \tag{7.9}$$

Assuming the most general initial condition, we define

$$p(k,v,\tau) = \int_{-\infty}^{\infty} dx\,e^{-ikx}\,p(x,v,\tau) \tag{7.10}$$

(spatial Fourier transform),

$$\tilde{p}(x,v,s) = \int_0^{\infty} d\tau\,e^{-s\tau}\,p(x,v,\tau) \tag{7.11}$$

(temporal Laplace transform),

$$\tilde{p}(k,v,s) = \int_0^{\infty} d\tau\,e^{-s\tau}\,p(k,v,\tau) \tag{7.12}$$

(Fourier–Laplace transform). Applying first the Fourier transform in the spatial variable we obtain

$$\left[\frac{\partial}{\partial\tau}+ikv+z(v)\right]p(k,v,\tau) = h_0(v)\int_{-\infty}^{\infty} du\,|v-u|\,p(k,u,\tau), \tag{7.13}$$

whence, by Laplace transformation and introduction of the new dependent variable

$$\tilde{f}(k,v,s) = \tilde{p}(k,v,s)/h_0(v), \tag{7.14}$$

we arrive at the pure integral equation

$$[z(v)+ikv+s]\,\tilde{f}(k,v,s) = \int_{-\infty}^{\infty} du\,|u-v|\,h_0(u)\,\tilde{f}(k,u,s)+\frac{p(k,v,0)}{h_0(v)}. \tag{7.15}$$

After differentiation twice with respect to velocity, this leads in turn to the singular differential equation

$$[z(v)+ikv+s]\,\tilde{f}''(k,v,s)+2[z'(v)+ik]\,\tilde{f}'(k,v,s) = [p(k,v,0)/h_0(v)]''. \tag{7.16}$$

(Here and throughout primes will be taken to refer to differentiation with respect to the velocity variable.)

We can see already the considerable simplification that results from the assumption of an initial distribution that is uncorrelated in position and velocity and has velocities equilibrated to $h_0(v)$. Avoiding this easier option, we next define the auxiliary function

$$\Omega(k, v, s) = z(v) + \mathrm{i}kv + s, \tag{7.17}$$

in terms of which the differential equation can be written

$$[\Omega(k, v, s)^2 \tilde{f}'(k, v, s)]' = \Omega(k, v, s)\,[p(k, v, 0)/h_0(v)]''. \tag{7.18}$$

Observing that this has an integrating factor $\Omega(k, v, s)$, the solution may be found directly in the form

$$\tilde{f}(k, v, s) = A(k, s) + B(k, s) \int_0^v \frac{\mathrm{d}u}{\Omega(k, u, s)^2} + 2\int_0^v \frac{\mathrm{d}u\,\gamma(k, u)}{\Omega(k, u, s)^2} + \frac{\gamma'(k, u)}{h_0(v)\,\Omega(k, v, s)}, \tag{7.19}$$

with $\gamma(k, v)$ conveniently defined by

$$\gamma(k, v) = \int_{-\infty}^{v} p(k, u, 0)\,\mathrm{d}u. \tag{7.20}$$

Here $A(k, s)$ and $B(k, s)$ are functions of integration still to be determined and we do not exclude the possibility that $p(k, v, 0)$ may be singular.

We now need to determine A and B by substitution of the solution (7.19) back into the integral equation (7.13), a process which evidently requires the evaluation of the following three integrals:

$$I_1 = \int_{-\infty}^{\infty} \mathrm{d}u\,|v-u|\,h_0(u) \int_0^u \frac{\mathrm{d}y}{\Omega(k, y, s)^2},$$

$$I_2 = 2\int_{-\infty}^{\infty} \mathrm{d}u\,|v-u|\,h_0(u) \int_0^u \frac{\mathrm{d}y\,\gamma(k, y)}{\Omega(k, y, s)^2},$$

$$I_3 = \int_{-\infty}^{\infty} \frac{\mathrm{d}u\,|v-u|\,p(k, u, 0)}{\Omega(k, u, s)^2}.$$

Defining now the further integral

$$U(k, v, s) = \int_0^v \frac{\mathrm{d}y}{\Omega(k, y, s)^2}, \tag{7.21}$$

and making use of the identities

$$\frac{\partial}{\partial v}\{[z'(v) + \mathrm{i}k]\,U(k, v, s) + \Omega(k, v, s)^{-1}\} = z''(v)\,U(k, v, s),$$

$$\frac{\partial}{\partial v}\{v\Omega(k, v, s)^{-1} - [z(v) - vz'(v) + s]\,U(k, v, s)\} = vz''(v)\,U(k, v, s),$$

together with $z''(v) = 2h_0(v)$ and $z'(\infty) = 1$, we arrive by now familiar partial integrations at the value of I_1:

$$I_1 = \Omega(k, v, s)\,U(k, v, s) - \tfrac{1}{2}v[(1+\mathrm{i}k)\,U(k, \infty, s) - (1-\mathrm{i}k)\,U(k, -\infty, s)] + \frac{1}{2}\left\{\frac{1}{1+\mathrm{i}k} - \frac{1}{1-\mathrm{i}k} - s[U(k, \infty, s) - U(k, -\infty, s)]\right\}. \tag{7.22}$$

The complex function $U(k, v, s)$, which is central to our final results, has the limiting value $U(0, v, s) = Y(v, s)$ (cf. (4.12)). We also note that, because of the symmetry $z(-v) = z(v)$, the combinations occurring above have the character of

$$\left.\begin{aligned} U(k, v, s) - U(k, -v, s) &= 2\,\mathrm{Re}\{U(k, v, s)\},\\ U(k, v, s) + U(k, -v, s) &= 2\,\mathrm{Im}\{U(k, v, s)\}.\end{aligned}\right\} \tag{7.23}$$

In describing the integrals I_2 and I_3 further simplifications will be necessary. We define the additional functions

$$V(k,v,s) = \int_0^v \frac{\mathrm{d}y\,\gamma(k,y)}{\Omega(k,y,s)^2}, \tag{7.24}$$

$$V_1(k,v,s) = \int_0^v \frac{\mathrm{d}y\,p(k,y,0)}{\Omega(k,y,s)^2}, \tag{7.25}$$

$$V_2(k,v,s) = \int_0^v \frac{\mathrm{d}y\,yp(k,y,0)}{\Omega(k,y,s)^2}. \tag{7.26}$$

These may be shown to satisfy the derivative properties

$$\frac{\partial}{\partial v}\left\{[z'(v)+\mathrm{i}k]\,V(k,v,s) - V_1(k,v,s) + \frac{\gamma(k,v)}{\Omega(k,v,s)}\right\} = z''(v)\,V(k,v,s)$$

and
$$\frac{\partial}{\partial v}\left\{\frac{v\gamma(k,v)}{\Omega(k,v,s)} - V_2(k,v,s) - [z(v)+vz'(v)+s]\,V(k,v,s)\right\} = vz''(v)\,V(k,v,s),$$

which, together with the limits $\gamma(-\infty) = 0$, $z'(\infty) = 1$, $\Omega(k,\infty,s)^{-1} = 0$ and

$$\lim_{v\to 0}\left[\frac{v\gamma(k,v)}{\Omega(k,v,s)}\right] = \frac{\gamma(\infty)}{1+\mathrm{i}k}$$

lead to the desired results. If we suppress for the moment the arguments k and s in the V-functions, the second of the required integrals can be shown to be

$$\begin{aligned} I_2 = {} & 2\Omega(v)\,V(v) - 2[vV_1(v) - V_2(v)] \\ & - v\left\{[V(\infty) - V(-\infty)] + \mathrm{i}k[V(\infty)+V(-\infty)] + \frac{\gamma(\infty)}{\Omega(v)} - [V_1(\infty)+V_1(-\infty)]\right\} \\ & + \frac{\gamma(\infty)}{1+\mathrm{i}k} - s[V(\infty)+V(-\infty)] - [V_2(\infty)+V_2(-\infty)]. \end{aligned} \tag{7.27}$$

Similarly we arrive at

$$I_3 = 2vV_1(v) - 2V_2(v) + [V_2(\infty)+V_2(-\infty)] - v[V_1(\infty)+V_1(-\infty)]. \tag{7.28}$$

The way to the solution of (7.13) is now clear. We substitute the expression (7.19) back into the integral equation using the above integrals and find for the left-hand side and right-hand side respectively the expressions

$$\Omega(k,v,s)\,[A(k,s) + B(k,s)\,U(k,v,s) + 2V(k,v,s)] + p(k,v,0)/h_0(v),$$

and
$$A(k,s)\,z(v) + B(k,s)\,I_1 + I_2 + I_3 + p(k,v,0)/h_0(v).$$

Since the function $z(v)$ cancels on both sides, it remains only to force a solution by equating the constant terms and those proportional to v to obtain two separate linear equations in the unknown functions $A(k,s)$ and $B(k,s)$. These are then straightforwardly solved. The results are cumbersome, but may be expressed as follows

$$B(k,s) = [sd(k,s) + \mathrm{i}kc(k,s)]/[sb(k,s) + \mathrm{i}ka(k,s)]; \tag{7.29}$$

$$A(k,s) = [a(k,s)\,B(k,s) - c(k,s)]/2s, \tag{7.30}$$

where $$a(k,s) = \frac{1}{1+\mathrm{i}k} - \frac{1}{1-\mathrm{i}k} - s[U(k,\infty,s) + U(k,-\infty,s)], \tag{7.31}$$

$$b(k,s) = [U(k,\infty,s) - U(k,-\infty,s)] + \mathrm{i}k[U(k,\infty,s) + U(k,-\infty,s)], \tag{7.32}$$

$$c(k,s) = 2s[V(k,\infty,s) + V(k,-\infty,s)] - \frac{2\gamma(\infty)}{1+\mathrm{i}k}, \tag{7.33}$$

$$d(k,s) = -2[V(k,\infty,s) - V(k,-\infty,s)] - 2\mathrm{i}k[V(k,\infty,s) + V(k,-\infty,s)]. \tag{7.34}$$

We recall that the combinations of U-functions imply the simplicity of the relations (7.23) and note that the V-functions behave likewise provided that the function $p(x,v,0)$ is of *even* parity in the velocity.

Equation (7.19) with the functions A and B interpreted through equations (7.29)–(7.34) thus constitutes a complete solution of the spatially inhomogeneous special Rayleigh model, to within inverse Fourier and Laplace transforms. As is clear from the structure of the above equations, little can be done to write explicit expressions in the space and time variables; nevertheless the above provides a direct algorithm for the computation of $p(x,v,\tau)$ at all times.

7.2. *Special cases of the spatially inhomogeneous solution*

The complexity of the above general result is somewhat more typographical than profound, as we shall see on examining the rich structure of special cases embodied in the equations. We shall first recover the Résibois result, applying to delta initial conditions then go on to examine an initial Maxwellian and the limit of spatial uniformity leading back to the results of § 4.

Case (i). *Uncorrelated initial distribution*

We need only note that, for an initial condition $p(x,v,0) = \rho(x)\,p(v,0)$, (7.3), for which then $p(k,v,0) = \tilde{\rho}(k)\,p(v,0)$, the above results hold with a simplified definition of the V-integrals. Indeed we can now write $V(k,v,s) = \tilde{\rho}(k)\;V(v,s)$ with

$$V(v,s) = \int_0^v \frac{\mathrm{d}u\,\gamma(u)}{\Omega(k,u,s)^2} \tag{7.35}$$

and $$\gamma(v) = \int_{-\infty}^v \mathrm{d}u\,p(u,0). \tag{7.36}$$

Note that, unlike for correlated initial conditions, we can here write $\gamma(\infty) = 1$ by normalization.

Case (ii). *Initial δ-distributions*

For the initial condition $p(x,v,0) = \delta(x)\,\delta(v-v_0)$, the above simplification applies with $\tilde{\rho}(k) = 1$ and
$$V(k,\infty,s) = \int_0^\infty \frac{\mathrm{d}u\,H(u-v_0)}{\Omega(k,u,s)^2} = U(k,\infty,s) - U(k,v_0,s). \tag{7.37}$$

If we then, without loss of generality, take $v_0 > 0$, it follows that $V(k,-\infty,s) = 0$. Reconstructing the solution above, the functions A and B are now more manageable and we can write

$$A(k,s) = \frac{[2s+(1+\mathrm{i}k)/(1-\mathrm{i}k)]\,[U(k,\infty,s) - U(k,v_0,s)] - [(1-\mathrm{i}k)/(1+\mathrm{i}k)]\,U(k,-\infty,s)}{s[U(k,\infty,s) - U(k,-\infty,s)] + 2k^2/(1+k^2)}, \tag{7.38}$$

$$-\tfrac{1}{2}B(k,s) = \frac{s[U(k,\infty,s) - U(k,v_0,s)] + \mathrm{i}k/(1+\mathrm{i}k)}{s[U(k,\infty,s) - U(k,-\infty,s)] + 2k^2/(1+k^2)}. \tag{7.39}$$

The solution with these values is identical with that obtained by Résibois (1978).

Case (iii). *Equilibrated initial velocities*

We consider now the important special case (7.6) in which the particles are initially equilibrated to $h_0(v)$ in velocity but spatially distributed with density $\rho(x)$. Returning to equations (7.16) and (7.18) it is clear that both become homogeneous by vanishing of the derivative on the right, with the consequence that the solutions take on the simpler form

$$\tilde{f}(k,v,s) = A(k,s) + B(k,s)\, U(k,v,s). \tag{7.40}$$

In addition since $p(x,v,0) = \rho(x)\, h_0(v)$ and $p(k,v,0) = \tilde{\rho}(k)\, h_0(v)$, we can write

$$\begin{aligned}\gamma(k,v) &= \tfrac{1}{2}\tilde{\rho}(k)\int_{-\infty}^{v} h_0(u)\,\mathrm{d}u\\ &= \tfrac{1}{2}\tilde{\rho}(k)\,[z'(v)+1],\end{aligned}$$

whence

$$\begin{aligned}V(k,\,\pm\infty,s) &= \tfrac{1}{2}\tilde{\rho}(k)\int_{0}^{\pm\infty}\mathrm{d}u\,\frac{z'(u)+1}{\Omega(k,u,s)^2}\\ &= \tfrac{1}{2}\tilde{\rho}(k)/(1+s)+\tfrac{1}{2}\tilde{\rho}(k)\,(1-\mathrm{i}k)\,U(k,\,\pm\infty,s).\end{aligned} \tag{7.41}$$

It follows that

$$V(k,\infty,s)-V(k,\,-\infty,s) = \tfrac{1}{2}\tilde{\rho}(k)\,(1-\mathrm{i}k)\,\mathrm{Re}\,[U(k,\infty,s)], \tag{7.42}$$

$$V(k,\infty,s)+V(k,\,-\infty,s) = \tilde{\rho}(k)/(1+s)+(1-\mathrm{i}k)\,\mathrm{Im}\,[U(k,\infty,s)], \tag{7.43}$$

with the use of the simplifications (7.23). On entering these expressions into (7.29)–(7.34) and writing (7.40) above, we obtain a solution equivalent to within scaling to that first given by Raval (1978). The case of an initial δ-distribution in position (7.7) is recovered on simply putting $\tilde{\rho}(k) = 1$ throughout.

Case (iv). *The spatially uniform solution*

Lastly we shall indicate how the above results reduce to the spatially uniform solution of § 7 on going to the limit $k \to 0$. Taking this limit in the expressions (7.31)–(7.34) we see that

$$\begin{aligned}a(0,s) &= -s[U(0,\infty,s)+U(0,\,-\infty,s)] = 0,\\ b(0,s) &= [U(0,\infty,s)-U(0,\,-\infty,s)] = 2Y(\infty,s),\\ c(0,s) &= 2s[V(0,\infty,s)+V(0,\,-\infty,s)]-2,\\ d(0,s) &= -2[V(0,\infty,s)-V(0,\,-\infty,s)],\end{aligned}$$

while

$$B(0,s) = \frac{d(0,s)}{b(0,s)} = -\frac{V(0,\infty,s)-V(0,\,-\infty,s)}{Y(\infty,s)}, \tag{7.44}$$

$$A(0,s) = -\frac{c(0,s)}{2s} = -[V(0,\infty,s)+V(0,\,-\infty,s)]+\frac{1}{s}. \tag{7.45}$$

These simplify further for the initial δ-distribution condition in velocity, for which we can write

$$B(0,s) = -[Y(\infty,s)-Y(v_0,s)]/Y(\infty,s), \tag{7.46}$$

$$A(0,s) = -[Y(\infty,s)-Y(v_0,s)]+1/s. \tag{7.47}$$

A careful analysis of the cases $v < v_0$ and $v > v_0$ then shows that the solution takes the form

$$\tilde{f}(0, v, s) = \frac{\delta(v-v_0)}{h_0(v)\,[z(v)+s]} + \frac{1}{s} - \int_{\max(v,\,v_0)}^{\infty} \frac{dy}{[z(y)+s]^2} - \int_{0}^{\min(v,\,v_0)} \frac{dy}{[z(y)+s]^2} + \left[\frac{Y(v,s)\,Y(v_0,s)}{Y(\infty,s)}\right]. \tag{7.48}$$

This is clearly equivalent upon inversion to the expression (4.16). The general case (4.15) follows by superposition.

7.3. *Space–time correlation functions*

While the above solutions contain, in effect, a complete description of the evolution of a Rayleigh test-particle ensemble in position–velocity space, various reduced quantities are also of interest, not least in making comparisons with other models for which explicit solutions are not available. The most important such function is the *Van Hove space–time correlation function* $G(x,\tau)$ defined as

$$G(x,\tau) = \int_{-\infty}^{\infty} dv\, p(x,v,\tau) \tag{7.49}$$

with the understanding that $p(x,v,0) = \delta(x)\,h_0(v)$ (Van Hove 1954, Vineyard 1958). The function $G(x,\tau)$ measures the probability that a particle released from the origin at time $\tau = 0$ will turn up in a distance element dx about x after a time τ has elapsed, irrespective of its velocity. Evidently $G(x,0) = \delta(x)$ and

$$\int_{-\infty}^{\infty} dx\, G(x,\tau) = 1 \quad \text{for all} \quad \tau.$$

(Note that the full-range variable $x \in (-\infty, +\infty)$ distinguishes the one-dimensional case, in which necessarily $G(-\infty,\tau) = G(x,\tau)$ for all time, from the more familiar parity of $G(\boldsymbol{r},\tau)$ in three dimensions.)

Usually $G(x,\tau)$ is available only through its transforms, the *intermediate scattering function* $\chi(k,\tau)$:

$$\chi(k,\tau) = \int_{-\infty}^{\infty} dv\, p(k,v,\tau) \tag{7.50}$$

and the *differential energy-transfer cross section* $S(k,\tau)$:

$$S(k,\omega) = \int_{-\infty}^{\infty} d\tau\, e^{-i\omega\tau}\,\chi(k,\tau), \tag{7.51}$$

both these being in certain cases experimentally measurable. In theoretical work a further function is conveniently defined, namely

$$Q(k,s) = \int_{0}^{\infty} d\tau\, e^{-s\tau}\,\chi(k,\tau) = \int_{-\infty}^{\infty} dv\,\tilde{p}(k,v,s), \tag{7.52}$$

from which evidently $S(k,\omega) = Q(k,i\omega) + Q(k,-i\omega)$.

Our interest in the above functions will be primarily in relation to other models and approximations, particularly the Gaussian approximation of Vineyard (1958) and the somewhat primitive 'instant thermalization' model of Bohm & Gross (1949) and Nelkin & Ghatak (1964).

We shall consider the function $Q(k,s)$ and obtain an explicit formula for it by direct integration of the solution for $f(k,v,\tau)$. Thus from the general form (7.19) we find that

$$\begin{aligned} Q(k,s) &= \int_{-\infty}^{\infty} du\, h_0(u)\,\tilde{f}(k,u,s) \\ &= \tfrac{1}{2}A(k,s)\int_{-\infty}^{\infty} du\, z''(u) + \tfrac{1}{2}B(k,s)\int_{-\infty}^{\infty} du\, z''(u)\,U(k,u,s) + \int_{-\infty}^{\infty} du\, z''(u)\,V(k,u,s), \end{aligned}$$

whence via the obvious partial integrations it emerges that

$$Q(k,s) = A(k,s)+\tfrac{1}{2}B(k,s)\left[(1+\mathrm{i}k)\,U(k,\infty,s)+(1-\mathrm{i}k)\,U(k,-\infty,s)\right] + (1+\mathrm{i}k)\,V(k,\infty,s)+(1-\mathrm{i}k)\,V(k,-\infty,s) \tag{7.53}$$

which, on entering the expressions for A and B, simplifies to

$$Q(k,s) = \frac{g(k,\infty)\,(1-\mathrm{i}k)\left[U(k,\infty,s)-U(k,-\infty,s)\right]+2\mathrm{i}k\left[V(k,\infty,s)-V(k,-\infty,s)\right]}{s\left[U(k,\infty,s)-U(k,-\infty,s)\right]+2k^2/(1+k^2)}. \tag{7.54}$$

Taking now the special case $p(x,v,0) = \delta(x)\,h_0(v)$, the V-functions reduce to U-functions as before with the result that

$$Q(k,s) = \frac{(1+k^2)\left[U(k,\infty,s)-U(k,-\infty,s)\right]}{s\left[U(k,\infty,s)-U(k,-\infty,s)\right]+2k^2/(1+k^2)}. \tag{7.55}$$

This can be written explicitly as

$$Q(k,s) = (1+k^2)\int_{-\infty}^{\infty}\frac{\mathrm{d}u}{[z(u)+\mathrm{i}ku+s]^2}\Bigg/\left\{s\int_{-\infty}^{\infty}\frac{\mathrm{d}u}{[z(u)+\mathrm{i}ku+s]^2}+\frac{2k^2}{1+k^2}\right\}, \tag{7.56}$$

and determines the Van Hove function (7.49) to within a numerical inversion.

7.4. *Spatial moments and the Gaussian approximation*

In previous work much attention has been given to the calculation of the spatial moments $\langle x^{2n}(\tau)\rangle$ of the Van Hove function $G(x,\tau)$ by operating with its moment generating function, namely the function $Q(k,s)$. Only the even moments need be considered, the odd ones vanishing by the symmetry of the initial condition. The moments and their Laplace transforms can thus be defined

$$\langle x^{2n}(\tau)\rangle = \int_{-\infty}^{\infty}\mathrm{d}x\,x^{2n}\,G(x,\tau) = (-1)^n\,(\partial^{2n}/\partial k^{2n})\,\chi(k,\tau)\,|_{k=0}, \tag{7.57}$$

and

$$\langle x^{2n}(s)\rangle = \int_0^{\infty}\mathrm{d}\tau\,\mathrm{e}^{-s\tau}\,\langle x^{2n}(\tau)\rangle = (-1)^n\,(\partial^{2n}/\partial k^{2n})\,Q(k,s)\,|_{k=0}. \tag{7.58}$$

7.4.1. *The second spatial moment* $\langle x^2(s)\rangle$

From equation (7.58) we have immediately

$$\langle x^2(s)\rangle = -\left[(\partial^2/\partial k^2)\,Q(k,s)\right]_{k=0}, \tag{7.59}$$

whence, by use of (7.56), after some algebra,

$$\langle x^2(s)\rangle = \frac{2}{s^2\,Q(\infty,s)}-\frac{2}{s}. \tag{7.60}$$

Now we have a check on the consistency of this result in the form of the two alternative expressions for the diffusion constant D_0 of § 5.4.1:

$$D_0 = \int_0^{\infty}S_v(\tau)\,\mathrm{d}\tau = \tfrac{1}{2}\lim_{\tau\to\infty}\frac{\partial}{\partial\tau}\langle x^2(\tau)\rangle \tag{7.61}$$

(see for example Desai & Nelkin 1966). Using the derivative and limit theorems for the Laplace transform

$$\mathscr{L}[(\partial/\partial\tau)\langle x^2(\tau)\rangle] = s\langle x^2(s)\rangle, \tag{7.62}$$

$$\lim_{s\to 0} s\tilde{f}(s) = \lim_{t\to\infty} f(\tau), \tag{7.63}$$

for the second expression in (7.61), we find

$$D_0 = \tfrac{1}{2}\lim_{s\to 0} s^2\langle x^2(s)\rangle$$

$$= \left[\int_0^\infty \frac{\mathrm{d}u}{z(u)^2}\right]^{-1}. \tag{7.64}$$

This is precisely the equation obtained earlier from the velocity autocorrelation function (equation (5.14)).

To obtain the actual second moment as a function of time we must evaluate the inverse $\mathscr{L}^{-1}\{[s^2 Y(0,s)]^{-1}\}$. Expressing this as the complex integral

$$\mathscr{L}^{-1}\{[s^2 Y(0,s)]^{-1}\} = \frac{1}{2\pi\mathrm{i}}\int_{\sigma-\mathrm{i}\infty}^{\sigma+\mathrm{i}\infty} \frac{\mathrm{d}s\,\mathrm{e}^{s\tau}}{s^2 Y(0,s)} \tag{7.65}$$

and replacing the path by the usual contour ABCDEF of figure 5, we see immediately that the occurrence of s^2 indicates a second-order pole at the origin. Calculating the residue, we find

$$\operatorname*{res}_{s=0}[\mathrm{e}^{s\tau}/s^2 Y(0,s)] = \frac{\tau}{Y(0,0)} + \frac{2}{Y(0,0)^2}\int_0^\infty \frac{\mathrm{d}u}{z(u)^3}. \tag{7.66}$$

The contributions of the arcs BC and FA vanishing as before, there remain only those from the integrals above and below the branch-cut. In similar manner to the development of § 4.2 we can write these as

$$\int_{\mathrm{CDEF}} \mathrm{d}s\,\mathrm{e}^{s\tau}/s^2\,Y(\infty,s) = 2\mathrm{i}\int_0^\infty \mathrm{d}v_\lambda\, z'(v_\lambda)\,\mathrm{e}^{-z(v_\lambda)\tau}\,\mathrm{Im}[B^-(\lambda)],$$

where

$$2\mathrm{i}\,\mathrm{Im}[B^-(\lambda)] = \lim_{\epsilon\to 0}\left\{\frac{1}{[-z(v_\lambda)-\mathrm{i}\epsilon]^2\,Y(\infty,\lambda-\mathrm{i}\epsilon)} - \frac{1}{[-z(v_\lambda)+\mathrm{i}\epsilon]^2\,Y(\infty,-\lambda+\mathrm{i}\epsilon)}\right\}$$

$$= \frac{2\pi\mathrm{i}\,g(\infty,\lambda)}{[R(\infty,\lambda)^2+\pi^2 g(\infty,\lambda)^2]\,z(v_\lambda)^2}.$$

From this we can deduce our final result that

$$\langle x^2(\tau)\rangle = 2D_0\tau - 2 + 4D_0\int_0^\infty \frac{\mathrm{d}u}{z(u)^3} + 2\int_0^\infty \frac{\mathrm{d}v_\lambda\, z'(v_\lambda)\,g(\infty,\lambda)\,\mathrm{e}^{-z(v_\lambda)\tau}}{z(v_\lambda)^2[R(\infty,\lambda)^2+\pi^2 g(\infty,\lambda)^2]}. \tag{7.67}$$

The non-Gaussian behaviour of the model is clearly seen in the last three terms, whose effect vanishes appropriately as $\tau\to\infty$. Moreover the structure of the fourth is precisely that needed to cancel the constant ones as $\tau\to 0$ and reproduce the correct initial condition $\langle x^2(0)\rangle = 0$. The asymptotic result $\langle x^2(\tau)\rangle \underset{\tau\to\infty}{\sim} 2D_0\tau$ is self-evident.

7.4.2. *The fourth spatial moment* $\langle x^4(\tau)\rangle$

The fourth spatial moment is of particular interest in that it can be used to provide a measure of deviations from Gaussian behaviour in the time-dependence of $G(x,\tau)$. The Gaussian approximation to $G(x,\tau)$ as introduced by Vineyard (1958) would require that, for the special Rayleigh model

$$G(x,\tau) = \pi^{\frac{1}{2}}\eta(\tau)^{-1}\exp[-x^2/\eta(\tau)^2], \tag{7.68}$$

with $\eta(\tau)$ a function to be determined. To the extent that this is the case we would expect to have

$$\frac{1}{3}\frac{\langle x^4(\tau)\rangle}{\langle x^2(\tau)\rangle^2} = 1 \tag{7.69}$$

for all times.

Now the Laplace transform of the fourth spatial moment is given by

$$\langle x^4(s)\rangle = (\partial^4/\partial k^4)\, Q(k, s)|_{k=0},$$

so that again the required quantity can be obtained by differentiation of the expression (7.56). After some lengthy manipulations followed by passage to the limit we find that

$$\langle x^4(s)\rangle = \frac{24}{Y(\infty, s)^2 s^2}\left[\frac{1}{s} - 3\int_0^\infty \frac{\mathrm{d}u\, u^2}{[z(u)+s]^4}\right]. \tag{7.70}$$

An alternative form, connected by an integration by parts is

$$\langle x^4(s)\rangle = \frac{72}{Y(\infty, s)^2 s^3}\int_0^\infty \frac{\mathrm{d}u\, u^2[z(u) - uz'(u)]}{[z(u)+s]^4}. \tag{7.71}$$

The correct limiting behaviour

$$\lim_{s\to\infty} s\langle x^4(s)\rangle = \lim_{\tau\to 0} \langle x^4(\tau)\rangle = 0$$

is again transparent.

Though it is possible to give a very complicated expression for $\langle x^4(\tau)\rangle$ by inversion of the above rather as for $\langle x^2(\tau)\rangle$, we shall rest content here with a numerical inversion-calculation designed to test the effectiveness of the Gaussian approximation for the Rayleigh model, using equation (7.71) as it stands. The results are given in the next section.

We can, however, examine the asymptotic behaviour of $\langle x^4(\tau)\rangle$ rather easily. From equation (7.71) we see that the contour for evaluating $\langle x^4(\tau)\rangle$ would skirt the usual branch-cut on the negative real axis and enclose a third-order pole at $s = 0$. From the limit theorems we have already used, we know that the dominant contribution at long times should come from the pole rather than from the cut. Thus we may assert that

$$\begin{aligned}\langle x^4(\tau)\rangle &\sim \operatorname*{res}_{s=0} \mathrm{e}^{s\tau}\langle x^4(s)\rangle, \quad \tau\to\infty,\\ &= \lim_{s\to 0} \tfrac{1}{2}(\mathrm{d}^2/\mathrm{d}s^2)\,[s^3\,\mathrm{e}^{s\tau}\langle x^4(s)\rangle]\\ &= \tfrac{1}{2}[\tau^2 + \tau(\mathrm{d}/\mathrm{d}s) + (\mathrm{d}^2/\mathrm{d}s^2)]\,\langle x^4(s)\rangle|_{s=0}.\end{aligned} \tag{7.72}$$

Defining the numerical quantities

$$\eta(n, m) = \int_0^\infty \frac{\mathrm{d}u\, u^m}{z(u)^n}, \quad m < n \tag{7.73}$$

and carrying out the necessary operations on equation (7.71) we find that

$$\langle x^4(\tau)\rangle \underset{\tau\to\infty}{\sim} 12D_0^2\tau^2 + C_1\tau + C_0, \tag{7.74}$$

where $C_1 = 12D_0^2[4D_0\eta(3,0) - 3\eta(4,2)]$,

$C_0 = 72D_0^2[D^2\eta(3,0) - 4D_0\eta(4,0) - 8D_0\eta(3,0)\,\eta(4,2) + 4\eta(5,2)]$.

7.5. *Numerical calculations on spatial moments*

To obtain the detailed behaviour of $\langle x^2(\tau)\rangle$ and $\langle x^4(\tau)\rangle$ for all times we used the Dubner–Abate inversion of the Laplace transforms $\mathscr{L}^{-1}[\langle x^2(s)\rangle]$ and $\mathscr{L}^{-1}[\langle x^4(s)\rangle]$ as described in § 4.4. At the same time we evaluated the constants C_0 and C_1 given after (7.4) using the expression (2.46) for $z(v)$ of the Maxwellian heat-bath.

The results of these calculations are illustrated in figures 12–14 over a time-range of zero to some 20 unit collision-times ($[z(0)]^{-1}$). In figure 12 the true second moment is compared with the asymptotic estimate $2D_0\tau$. It will be seen that $\langle x^2(\tau)\rangle$ is exceedingly linear for $\tau > 2$, with the asymptotic estimate quite adequate at times beyond this value. A similar correspondence will be found for the fourth moment (figure 13), except that here $\langle x^4(\tau)\rangle$ is quite seriously falsified by the asymptotic approximation at shorter times.

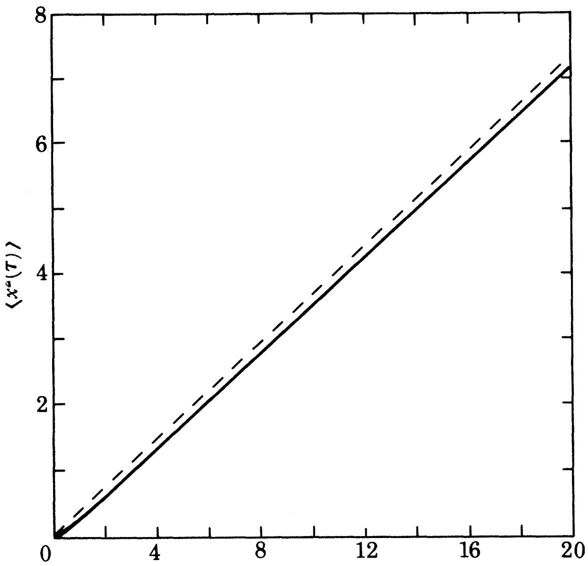

FIGURE 12. Time evolution of the second spatial moment $\langle x^2(\tau)\rangle$ for an initially localized Maxwellian distribution of Rayleigh test-particles. The dashed line represents the asymptotic value $\langle x^2(\tau)\rangle \sim 2D_0\tau$.

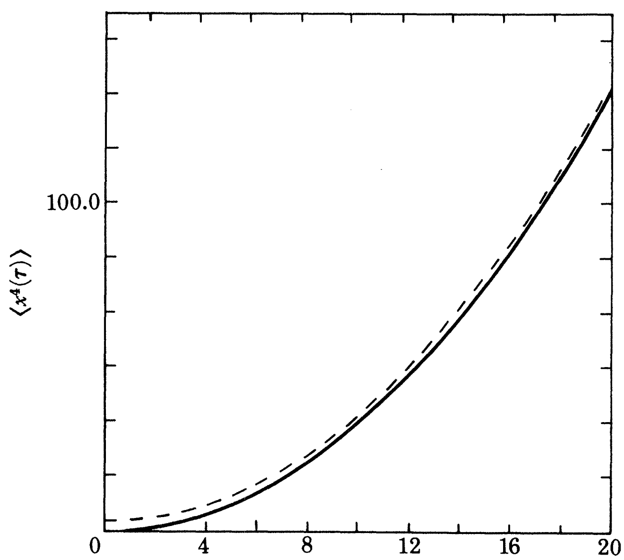

FIGURE 13. Time evolution of the fourth spatial moment $\langle x^4(\tau)\rangle$ of an initially localized Maxwellian distribution. The dashed line is the asymptotic result (7.74).

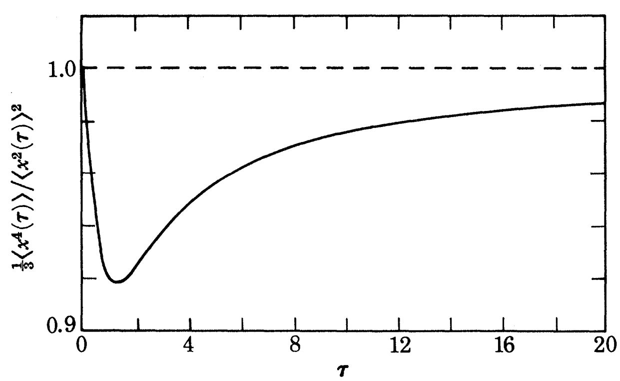

FIGURE 14. Ratio of the moments $3\langle x^2(\tau)\rangle^2/\langle x^4(\tau)\rangle$. The value is unity for truly Gaussian behaviour; in fact for the Rayleigh model such behaviour is limited to very short and very long times.

Lastly, in figure 14 we compute the ratio of moments $3\langle x^2(\tau)\rangle^2/\langle x^4(\tau)\rangle$ as a measure of deviation from Gaussian behaviour. The departure is indeed considerable and characteristically greater in the medium-time regime $0.5 < \tau < 5$, the maximum discrepancy being at $\tau = 0.9$ collision times. This behaviour is broadly similar to that found by Nelkin & Ghatak (1964) for the Bohm–Gross model (Bohm & Gross 1949).

We may reasonably conclude that, so far as the special Rayleigh model is concerned, the Gaussian approximation to the Van-Hove correlation function $G(x, \tau)$ is not to be taken as more than a rough guide to the general shape of the space–time correlation. Such discrepancy, like that found by Nelkin & Ghatak, should probably be regarded as the rule rather than the exception in particle transport statistics.

8. Conclusion

While we have attempted to make this a definitive study of the special Rayleigh model, we have not gone to all possible lengths to cover every aspect of interest. In particular we have not considered the interesting problems that arise when *spatial* absorbing or reflecting barriers are introduced and where sources may also be present. These refinements, which are more in the spirit of neutron and radiative transport theory, are undoubtedly non-trivial in one dimension, but their study would have taken us too far afield. We have also neglected to treat the eigenvalue problem underlying the spatially inhomogeneous model, in which the occurrence of complex eigenvalues of the form $\lambda = z(v_\lambda) \pm ikv_\lambda$ lends an element of wave-like character to the solutions and requires us to express the solution for $p(k, v, \tau)$ as an integral in a complex λ-plane. While a sufficiently ingenious use of this formulation might lead, as in the spatially homogeneous case, to a useful alternative to the transform solutions, evidence from neutron transport theory (see for example Corngold 1964) shows the problem to be of considerable complexity and we have not succeeded in carrying it beyond formal expressions. These are no real alternative to the comparatively explicit solutions given in § 7.

In concluding we cannot but return momentarily to the *general* Rayleigh problem in which the test-particles have mass distinct from but comparable with that of the heat-bath particles (Hoare & Rahman 1973). Although in this case the scattering kernel remains relatively simple in form, its spectral properties are undoubtedly far more complex both in the discretum and continuum branches than those elucidated here. While a certain amount is known about the passage to the Brownian motion limit, and recent numerical calculations have thrown light on the nature of the discrete spectrum (Barker *et al.* (1981)) virtually no progress has been made in analysing the continuum and its role in the relaxation process. This problem is evidently of an order of difficulty such that our lengthy studies of the unit-mass-ratio model still give scarcely a hint of how an analytic solution to the general model might be sought.

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Appendix 1. Calculus of elementary discontinuous functions

We collect here and illustrate the main properties of the discontinuous functions introduced in § 3, with particular reference to their decomposition into parity components. The operations written here are, of course, 'symbolic', but can be justified in the context of distribution theory in the usual manner.

A 1.1. *The elementary discontinuous functions*

We consider the five functions of the two variables x and y. In most operations x is considered the variable of interest and the functions are essentially undefined for $x = y$.

			$x<y$	$x>y$
(i)	$\lvert x-y\rvert$	$=$	$y-x$	$x-y$
(ii)	$\max(x,y)$	$=$	y	x
(iii)	$\min(x,y)$	$=$	x	y
(iv)	$H(x-y)$	$=$	0	1
(v)	$\operatorname{sgn}(x-y)$	$=$	-1	1

A 1.2. *Derivative relations*

$$(a)\quad (\mathrm{d}/\mathrm{d}x)\,|x-y| = \operatorname{sgn}(x-y) = 2H(x-y)-1, \tag{A 1.1}$$

$$(b)\quad (\mathrm{d}/\mathrm{d}x)\max(x,y) = H(x-y), \tag{A 1.2}$$

$$(c)\quad (\mathrm{d}/\mathrm{d}x)\min(x,y) = H(x-y)-1, \tag{A 1.3}$$

$$(d)\quad (\mathrm{d}/\mathrm{d}x)\,H(x-y) = \delta(x-y), \tag{A 1.4}$$

$$(e)\quad (\mathrm{d}/\mathrm{d}x)\operatorname{sgn}(x-y) = 2\delta(x-y). \tag{A 1.5}$$

A 1.3. *Parity decomposition*

(*a*) *The modulus function*

Let
$$|x-y| = |x-y|_{\mathrm{ev}} + |x-y|_{\mathrm{od}}; \quad (x \neq y),$$
then
$$|x-y|_{\mathrm{ev}} = \tfrac{1}{2}(|x-y|+|x+y|) = \max(x,y), \tag{A 1.6}$$
$$|x-y|_{\mathrm{od}} = \tfrac{1}{2}(|x-y|-|x+y|) = -\operatorname{sgn}(x)\operatorname{sgn}(y)\min(|x|,|y|). \tag{A 1.7}$$

On differentiation the components behave as follows:

$$\begin{aligned}(\mathrm{d}/\mathrm{d}x)\,|x-y|_{\mathrm{ev}} &= [(\mathrm{d}/\mathrm{d}|x|)\max(|x|,|y|)]\,(\mathrm{d}|x|/\mathrm{d}x)\\ &= \operatorname{sgn}(x)\,H(|x|-|y|)\\ &= H(x+y)+H(x-y)-1,\end{aligned} \tag{A 1.8}$$

and
$$\begin{aligned}(\mathrm{d}/\mathrm{d}x)\,|x-y|_{\mathrm{od}} &= -2\delta(x)\operatorname{sgn}(y)\min(|x|,|y|)\\ &\quad -\operatorname{sgn}(x)^2\operatorname{sgn}(y)\,[H(|x|-|y|)-1]\\ &= -\operatorname{sgn}(y)\,[H(|x|-|y|)-1].\end{aligned} \tag{A 1.9}$$

Similarly
$$\begin{aligned}(\mathrm{d}^2/\mathrm{d}x^2)\,|x-y|_{\mathrm{ev}} &= \operatorname{sgn}(x)\,\delta(|x|-|y|)\\ &= \delta(x+y)+\delta(x-y) = 2\delta(x-y)_{\mathrm{ev}},\end{aligned} \tag{A 1.10}$$

and
$$(\mathrm{d}^2/\mathrm{d}x^2)\,|x-y|_{\mathrm{od}} = -\operatorname{sgn}(x)\operatorname{sgn}(y)\,\delta(|x|-|y|) = 2\delta(x-y)_{\mathrm{od}}. \tag{A 1.11}$$

Note that in each case the ordinary derivative relations are recovered on combining the appropriate parity components.

(*b*) *The Heaviside function*

If
$$H(x-y) = H_{\mathrm{ev}}(x-y) + H_{\mathrm{od}}(x-y)$$
then
$$H_{\mathrm{ev}}(x-y) = \tfrac{1}{2}\{1-\operatorname{sgn}(y)\,[H(|x|-|y|)-1]\}, \tag{A 1.12}$$
$$H_{\mathrm{od}}(x-y) = \tfrac{1}{2}\operatorname{sgn}(x)\,H(|x|-|y|). \tag{A 1.13}$$

(*c*) *The δ-function*

If
$$\delta(x-y) = \delta_{\mathrm{ev}}(x-y) + \delta_{\mathrm{od}}(x-y),$$
then
$$\delta_{\mathrm{ev}}(x-y) = \tfrac{1}{2}[\delta(x-y)+\delta(x+y)] = \delta(|x|-|y|), \tag{A 1.14}$$
$$\delta_{\mathrm{od}}(x-y) = \tfrac{1}{2}[\delta(x-y)-\delta(x+y)] = -\operatorname{sgn}(x)\operatorname{sgn}(y)\,\delta(|x|-|y|). \tag{A 1.15}$$

These results may be represented graphically as in figure 15.

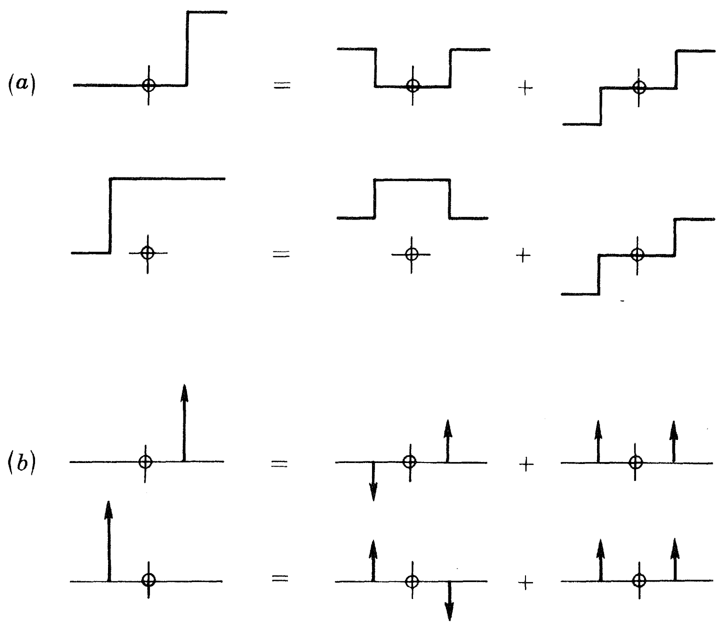

FIGURE 15. (*a*) Parity decomposition of the Heaviside step-function $H(x-y)$ for $y > 0$ (upper) and $y < 0$ (lower) (equations (A 1.13) and (A 1.14)). (*b*) Parity decomposition of the δ-function $\delta(x-y)$ for $y > 0$ (upper) and $y < 0$ (lower) (equations (A 1.15) and (A 1.16)).

APPENDIX 2. SOME REGULAR INTEGRALS

Three types of integral that occur repeatedly throughout the text are

$$J_1 = \int_0^\infty \mathrm{d}v\, h_0(v) R(v,\lambda) = R(\infty,\lambda) + \frac{1}{1-\lambda}, \tag{A 2.1}$$

$$J_2 = \int_0^\infty \mathrm{d}v\, v h_0(v)\, R(v,\lambda) = 1 + \lambda R(\infty, \lambda), \tag{A 2.2}$$

$$J_3 = \int_0^\infty \mathrm{d}v\, h_0(v)\, R(v,\lambda)\, R(v,\lambda') = R(\infty,\lambda)\, R(\infty,\lambda') + \frac{1}{\lambda'-\lambda}[R(\infty,\lambda) - R(\infty,\lambda')], \tag{A 2.3}$$

where as throughout $$R(v,\lambda) = \int_0^v \frac{\mathrm{d}y}{[z(y)-\lambda]^2},$$

and we confine our attention for the present to the *regular* range of λ, namely $\lambda \notin [1,\infty]$ on the real line. The above results are consequent upon the special properties of the functions h_0 and z, those relevant here being

(*a*) $z(0) = 1$, (*b*) $z'(0) = 0$,

(*c*) $z(\pm\infty) = \infty$, (*d*) $z'(\pm\infty) = \pm 1$,

(*e*) $2h_0 = z''$, (*f*) $vz' - z \to 0$ as $v \to \pm\infty$.

Using first (*e*) we have for J_1:

$$2J_1 = z' \int_0^v \frac{\mathrm{d}y}{[z-\lambda]^2}\bigg|_0^\infty - \int_0^\infty \frac{\mathrm{d}v\, z'}{[z-\lambda]^2}$$
$$= \int_0^\infty \frac{\mathrm{d}y}{[z-\lambda]^2} + \frac{1}{z-\lambda}\bigg|_0^\infty.$$

The above result follows on using (*a*) and (*c*) in the last term.

Consider now the integral J_2. Noting that $vz'' = (vz')' - z'$ we can write

$$J_2 = \int_0^\infty \mathrm{d}v \left[\frac{\mathrm{d}}{\mathrm{d}v}(vz'-z)\right] \int_0^v \frac{\mathrm{d}y}{[z(y)-\lambda]^2}$$
$$= (vz'-z) \int_0^v \frac{\mathrm{d}y}{(z-y)^2}\bigg|_0^\infty - \int_0^\infty \frac{\mathrm{d}v(vz'-z)}{(z-\lambda)^2}.$$

Thus, since the boundary terms vanish by (*f*) above,

$$J_2 = \int_0^\infty \mathrm{d}v\, v \frac{\mathrm{d}}{\mathrm{d}v}\left(\frac{1}{z-\lambda}\right) - \int_0^\infty \frac{\mathrm{d}v}{z-\lambda} + \int_0^\infty \frac{\mathrm{d}v\, z}{(z-\lambda)^2}.$$

Putting now $z = (z-\lambda) + \lambda$ in the numerator of the last integral, the second term cancels and on evaluating the first by parts $$J_2 = \frac{v}{z-\lambda}\bigg|_0^\infty + \lambda \int_0^\infty \frac{\mathrm{d}y}{(z-\lambda)^2}.$$

Using then (*f*) for the upper limit of the first term, the result (A 2.2) follows.

Turning now to the integral J_3 we see that

$$2J_3 = \int_0^\infty z''\, R(v,\lambda)\, R(v,\lambda')$$
$$= z'(v)\, R(v,\lambda)\, R(v,\lambda')|_0^\infty - \int_0^\infty \mathrm{d}v\, z' \left[\frac{R(v,\lambda)}{(z-\lambda')^2} + \frac{R(v,\lambda')}{(z-\lambda)^2}\right]$$
$$= R(\infty,\lambda)\, R(\infty,\lambda') + \left[\frac{R(v,\lambda)}{z-\lambda'} + \frac{R(v,\lambda')}{z-\lambda}\right]\bigg|_0^\infty - \int_0^\infty \mathrm{d}v \left[\frac{1}{(z-\lambda')(z-\lambda)^2} + \frac{1}{(z-\lambda)(z-\lambda')^2}\right].$$

A partial-fraction decomposition of the remaining integrand shows that

$$\left[\frac{1}{(z-\lambda')(z-\lambda)^2} + \frac{1}{(z-\lambda)(z-\lambda')^2}\right] = \frac{1}{\lambda-\lambda'}\left[\frac{1}{(z-\lambda)^2} - \frac{1}{(z-\lambda')^2}\right].$$

Since the boundary terms vanish, the result (A 2.3) follows immediately.

The various complex integrals occurring in § 5 can be treated in the same manner on putting $\lambda = -s$ in the above, provided always that s is not on the branch-cut extending from -1 to $-\infty$ on the negative real axis. Several similar integrals with limits other than 0 to ∞ have occurred; these are closely related to the above and may be treated similarly with obvious changes in the boundary terms.

Appendix 3. Pseudofunctions and Hadamard finite parts

Here we shall examine briefly the interpretation of the pseudofunction $\mathrm{Pf}\,R(v, \lambda)$ which occurs either alone or in integrals of the previous types when the quantity $[z(v)-\lambda]^{-1}$ possesses a singularity in the range of integration. We write

$$R(v, \lambda) = \mathrm{Pf}\int_0^v \frac{\mathrm{d}y}{[z(y)-\lambda]^2}, \tag{A 3.1}$$

as in (3.7) it being now understood that $\lambda \in [1, \infty]$ and $z(v) \in [0, \infty]$. The sense of the above is that we need to interpret inner products of the form $\langle \mathrm{Pf}\,R(v, \lambda), \phi(v)\rangle$ for suitable test-functions ϕ as

$$\langle \mathrm{Pf}\,R(v, \lambda), \phi(v)\rangle = \mathrm{Fp}\int_a^b \mathrm{d}v\, R(v, \lambda)\, \varphi(v). \tag{A 3.2}$$

Here the prefix Fp on the right indicates the extraction of the Hadamard finite part of the formally divergent integral appearing there. This process will now be illustrated.

Since by definition of the derivative of a distribution:

$$\langle \mathrm{Pf}\,R(v, \lambda), \varphi'(v)\rangle = -\langle \mathrm{Pf}[z(v)-\lambda]^{-2}, \varphi(v)\rangle \tag{A 3.3}$$

we can modify the set of test-functions and concentrate on the interpretation of

$$\langle \mathrm{Pf}[z(v)-\lambda]^{-2}, \varphi(v)\rangle = \mathrm{Fp}\int_a^b \frac{\mathrm{d}v\,\varphi(v)}{[z(v)-\lambda]^2}. \tag{A 3.4}$$

After Hadamard (see especially Zemanian 1965, §§ 1.4 and 2.5) we put

$$\langle \mathrm{Pf}[z-\lambda]^{-2}, \varphi\rangle = \lim_{\epsilon_v \to 0}\left\{\left(\int_a^{v_\lambda - \epsilon_v} + \int_{v_\lambda+\epsilon_v}^b\right)\frac{\mathrm{d}v\,\varphi(v)}{[z(v)-\lambda]^2} - I(\epsilon_v)\right\},$$

where $I(\epsilon_v)$ is an infinite part to be determined. As always we write $z(v_\lambda) = \lambda$.

It is convenient first to change to an integral over z, writing $F(z) = \phi[v(z)]/(\mathrm{d}z/\mathrm{d}v)$ and letting the limit quantity change such that $\epsilon_z = z'(v)\,\epsilon_v$. In these terms we can write

$$\langle \mathrm{Pf}[z-\lambda]^{-2}, \varphi\rangle = \lim_{\epsilon_z \to 0}\left\{\left(\int_{z(a)}^{\lambda - \epsilon_z} + \int_{\lambda+\epsilon_z}^{z(b)}\right)\frac{\mathrm{d}z\,F(z)}{[z-\lambda]^2} - I(\epsilon_z)\right\}.$$

The function $F(z)$ is now expanded about the point $z = \lambda$ to an order sufficient to remove the singularity. Thus

$$F(z) = F(\lambda) + F'(\lambda)\,(z-\lambda) + \psi(z)\,(z-\lambda)^2,$$

where $\psi(z)$ is a function, regular at $z = \lambda$ which need not be determined. On inserting this expression into the integrals and evaluating we find that

$$\langle \mathrm{Pf}[z-\lambda]^{-2}, \varphi\rangle = F(\lambda)\left(\frac{1}{z(a)-\lambda} - \frac{1}{z(b)-\lambda}\right) + F'(\lambda)\ln\left[\frac{z(b)-\lambda}{z(a)-\lambda}\right]$$
$$+ \int_{z(a)}^{z(b)} \mathrm{d}z\,\psi(z) + \lim_{\epsilon_z \to 0}\left[\frac{2F(\lambda)}{\epsilon_z} - I(\epsilon_z)\right],$$

the logarithmic terms in ϵ_z having cancelled. Thus it is clear that the infinite part of the integral is $I(\epsilon_z) = 2F(\lambda)/\epsilon_z$. Subtracting this according to the Hadamard prescription, we can therefore write

$$\langle \mathrm{Pf}[z-\lambda]^{-1}, \varphi\rangle = \lim_{\epsilon_z\to 0}\left\{\left(\int_{z(a)}^{\lambda-\epsilon_z} + \int_{\lambda+\epsilon_z}^{z(b)}\right)\frac{F(z)\,\mathrm{d}z}{[z-\lambda]^2} - \frac{2F(\lambda)}{\epsilon_z}\right\}.$$

To return to the v-integration, we must remember that $\epsilon_z = z'(v_\lambda)\,\epsilon_v$, so that

$$\langle \mathrm{Pf}[z-\lambda]^{-2}, \varphi\rangle = \lim_{\epsilon_v\to 0}\left\{\left(\int_{a}^{v_\lambda-\epsilon_v} + \int_{v_\lambda+\epsilon_v}^{b}\right)\frac{\varphi(v)\,\mathrm{d}v}{[z(v)-\lambda]^2} - \frac{2\varphi(v_\lambda)}{\epsilon_v z'(v_\lambda)^2}\right\}. \qquad (\mathrm{A}\,3.5)$$

Although this expression is meaningful as it stands and might be used in numerical computations, we may use a simple trick to turn it into a form in which ϵ_z does not appear explicitly. Note that the equivalence

$$\left(\int_{a}^{v_\lambda-\epsilon_v} + \int_{v_\lambda+\epsilon_v}^{b}\right)\frac{\mathrm{d}v}{(v-v_\lambda)^2} = \frac{2}{\epsilon_v} - \left(\frac{1}{v_\lambda-a} + \frac{1}{b-v_\lambda}\right)$$

enables us to write

$$\langle \mathrm{Pf}[z-\lambda]^{-2}, \varphi\rangle = \int_a^b \mathrm{d}v\left\{\frac{\varphi(v)}{[z(y)-\lambda]^2} - \frac{\varphi(v_\lambda)}{z'(v_\lambda)^2\,(v-v_\lambda)^2}\right\} - \frac{\varphi(v_\lambda)}{z'(v_\lambda)^2}\left[\frac{b-a}{(v_\lambda-a)\,(b-v_\lambda)}\right]. \qquad (\mathrm{A}\,3.6)$$

An explicit form of the function $\mathrm{Pf}\,R(v,\lambda)$ can be obtained from the above by substituting $a = 0$ and $\varphi(y) = H(y)\,H(v-y)$. It follows straightforwardly that

$$\mathrm{Pf}\,R(v,\lambda) = \int_0^v \mathrm{d}y\left\{\frac{1}{[z(y)-\lambda]^2} - \frac{1}{z'(v_\lambda)^2\,(y-v_\lambda)^2}\right\} - \frac{1}{z'(v_\lambda)^2}\left[\frac{1}{v-v_\lambda} + \frac{1}{v_\lambda}\right] \quad (v > 0). \qquad (\mathrm{A}\,3.7)$$

This important relation allows us to separate the pseudofunction $R(v,\lambda)$ into regular and singular parts as we did in § 3.4 (equations (3.70) and (3.71)). The singular part giving only Cauchy principal values when integrated, only these need arise when inner products with $R(v,\lambda)$ are evaluated. Use of the above is thus an alternative to the application of the equivalence (A 3.3) above. Moreover integrals of products of Pf R pseudofunctions can be reduced to double Cauchy principal value integrals to which the Poincaré–Bertrand theorem applies.

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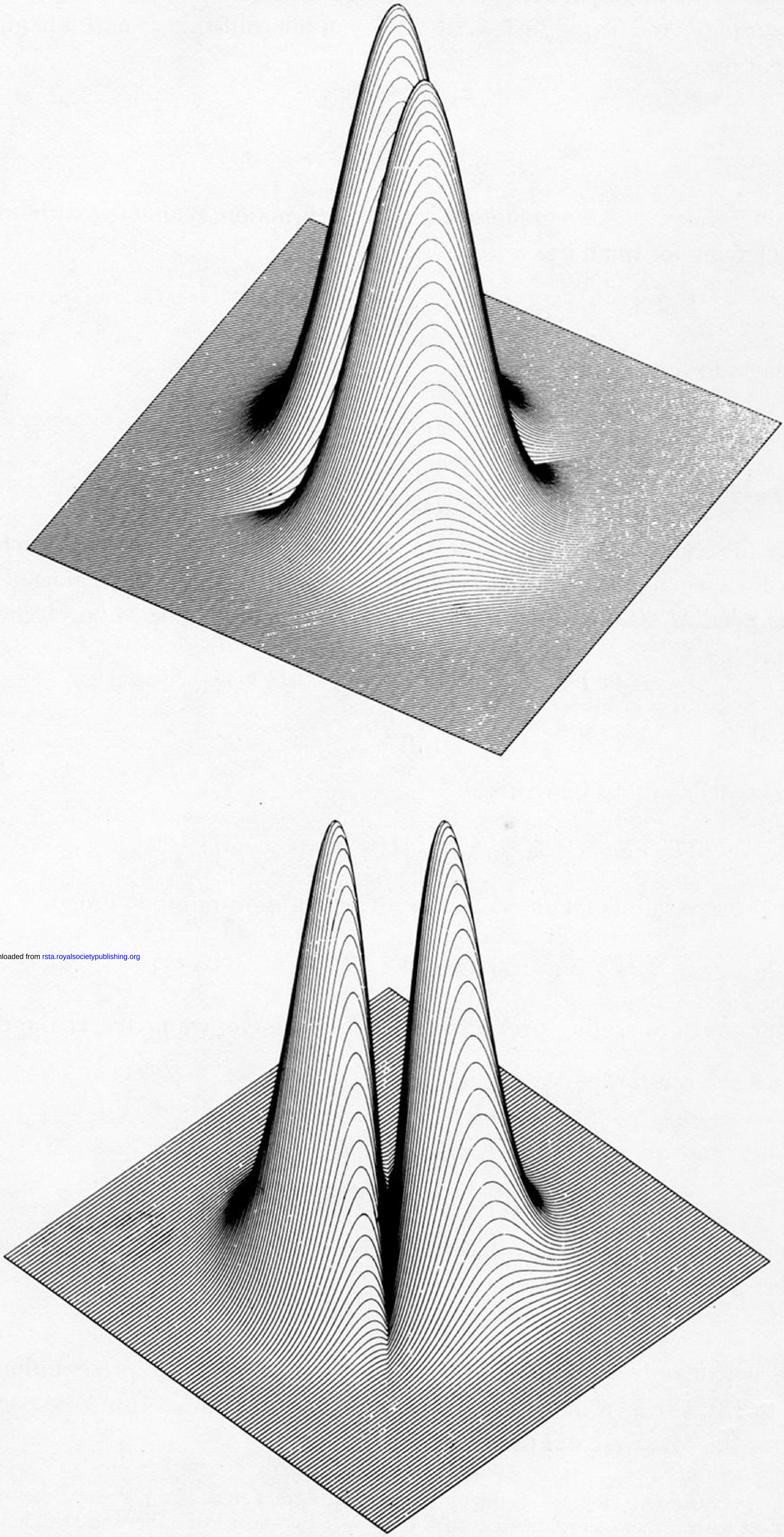

GURE 3. The symmetrized Rayleigh transition kernel $G(u, v)$ for a Maxwellian heat-bath (equations (2.18) and (2.45)). The coordinate origin of the u,v-plane is at the centre of the figure, the $u = v$ diagonal running between the peaks. Note the discontinuity in the first derivative along this line.

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