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On the spectral theory of Rayleigh's piston II. The exact singular solution for unit mass ratio

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Abstract. We have solved exactly the singular eigenvalue problem governing the relaxation of velocity for a one-dimensional ensemble of test particles in a heat bath of similar objects. This corresponds to the special case of Rayleigh's piston with mass ratio unity.

The eigenfunctions prove to be singular schwartzian distributions involving a combination of delta functions and Hadamard pseudofunctions. No discrete eigenvalues occur other than the isolated point $\lambda = 0$, and, correspondingly, no regular eigenfunctions other than the equilibrium maxwellian, to which the whole continuum set is orthogonal. The singular eigenfunctions divide naturally into even and odd subsets such that the former, involving only delta functions, govern the half-range problem for the evolution of the *speed* rather than the velocity ensemble, while the latter express all directional information.

Orthogonality and completeness relations are established and the initial-value problem for the relaxation of an initial δ ensemble is considered. Speed relaxation proves relatively simple and a closed form can be derived for the time-dependent distribution function. Velocity relaxation is considerably more complex, but can be specified in terms of standard solutions to a Carleman-type integral equation.

1. Introduction

The general Rayleigh model, which we described and began to investigate in part I of this series (Hoare and Rahman 1973) leads, for all its apparent simplicity, to a number of delicate mathematical problems. One surprising turn which our investigations have taken is the discovery that, in the simplest special case, where the masses of test particles and heat-bath particles are put equal, an exact solution to the singular eigenvalue problem may be obtained, which involves a quite unfamiliar combination of ordinary and generalized functions.

Since this both serves as an introduction to the complexities of the problem at general mass ratio and is also of interest in its own right as a rare and possibly unique example of an exactly-soluble singular master equation, we shall treat it here in some detail before continuing with what will necessarily be a more qualitative account of the full model.

Other types of one-dimensional gas model have recently attracted considerable attention, particularly through the work of Jepsen (1965) and Lebowitz *et al* (1968). Although these models also lead to exact solutions, it should be stressed that they are entirely different from the Rayleigh model studied here inasmuch as they treat the strictly N-body problem of non-penetrating rods constrained on a line, with full allowance

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for correlation in successive collisions—yet no possibility of velocity relaxation or dissipation of energy in a heat bath.

2. The equal mass model

We consider the special case of an ensemble of Rayleigh pistons responding to a heat bath of particles having identical mass M, ie our system consists of a labelled test particle in a one-dimensional gas without position or velocity correlations (figure 1). As before, attention is restricted to the spatially-homogeneous case and we seek primarily the solution of the initial-value problem for $P(V, t)$ the time-dependent velocity distribution function for the ensemble.

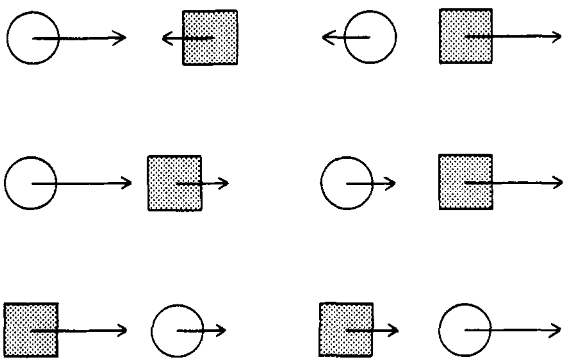

Figure 1. The Rayleigh piston at unit mass ratio. Test particles (shaded) and heat-bath particles collide in one dimension, their velocities before (left) and after (right) becoming interchanged. Collisions are of three types: A, 'head-on'; B, 'knocked-on'; C, 'knocking-on'; the relative probabilities of each changing with test-particle velocity. Collisions B and C as drawn above are *inverse* to each other.

The masses of all particles being equal, a considerably simplified kernel is obtained for the probability flux in transitions from velocity V to velocity in dV' about V'. We find (cf equation (2.4) of I):

$$K(V, V') = n\sigma\left(\frac{M}{2\pi k_B T}\right)^{1/2}|V-V'|\exp\left(-\frac{MV'^2}{2k_B T}\right) = n\sigma|V-V'|f_M(V') \quad (2.1)$$

where n is the number density of heat-bath particles, σ is the test-particle cross section, M is the mass of both system and heat-bath particles, T is the temperature of the heat bath, and $f_M(V)$ is the one-dimensional maxwellian for mass M.

Given the well known result that equal mass particles in one dimension simply exchange their respective velocities on collision, the form of the kernel becomes virtually self-evident. In terms of individual collisions (though not, of course, the ensemble as a whole) this simple mechanism may be thought of as a process of 'instant thermalization'.

The initial-value problem consists, as before, in obtaining time-dependent solutions $P(V, t)$ of the master equation:

$$\frac{\partial P(V,t)}{\partial t} = \int_{-\infty}^{+\infty} K(V', V)P(V', t)\,\mathrm{d}V' - Z(V)P(V,t) \tag{2.2}$$

with $P(V, 0)$ a specified initial distribution for the test-particle velocities. The velocity-dependent collision number $Z(V)$, in which the mass M enters only through the heat-bath maxwellian, can be written

$$Z(V) = n\sigma\left\{V\,\mathrm{erf}\left[\left(\frac{M}{2k_\mathrm{B}T}\right)^{1/2} V\right] + \left(\frac{2k_\mathrm{B}T}{\pi M}\right)^{1/2}\exp\left(-\frac{MV^2}{2k_\mathrm{B}T}\right)\right\}. \tag{2.3}$$

Again it is convenient to scale velocities and time in terms of the reduced variables

$$\begin{aligned} x &= (M/2k_\mathrm{B}T)^{1/2}V \\ y &= (M/2k_\mathrm{B}T)^{1/2}V' \\ \tau &= n\sigma(2k_\mathrm{B}T/\pi M)^{1/2}t. \end{aligned} \tag{2.4}$$

A further modification of the dependent variable

$$h(x,\tau) = P(x,\tau)\,\mathrm{e}^{\frac{1}{2}x^2} \tag{2.5}$$

leads to the self-adjoint form of the transport equation

$$\frac{\partial h(x,\tau)}{\partial \tau} = \int_{-\infty}^{+\infty} g(x,y)h(y,\tau)\,\mathrm{d}y - z(x)h(x,\tau) \tag{2.6}$$

in which $g(x, y)$ is the symmetric kernel:

$$g(x,y) = |x-y|\exp[-\tfrac{1}{2}(x^2+y^2)], \tag{2.7}$$

and $z(x)$ is the reduced collision number function:

$$z(x) = \exp(-x^2) + \pi^{1/2}x\,\mathrm{erf}(x). \tag{2.8}$$

We now seek solutions by a separation of variables in the form,

$$h(x,\tau) = \phi(x)\,\mathrm{e}^{-\lambda\tau} \tag{2.9}$$

and in this way are led to the singular eigenvalue problem

$$[z(x)-\lambda]\phi(x,\lambda) = \int_{-\infty}^{+\infty} g(x,y)\phi(y,\lambda)\,\mathrm{d}y. \tag{2.10}$$

The singular character arises not from the integral but from the term $[z(x)-\lambda]$ which may evidently vanish for combinations of x and λ when $1 \leqslant \lambda < \infty$. To make this more explicit, the eigenvalue condition can be written

$$\mathscr{H}\phi(x,\lambda) = \lambda\phi(x,\lambda)$$

where $\mathscr{H}$ stands for the singular integral operator with kernel†

$$H(x,y) = z(x)\delta(x-y) - g(x,y). \tag{2.11}$$

† In this context the function $z(x)$ is sometimes referred to as a 'multiplicative operator' (see eg Cercignani 1969, Tokizawa 1970).

The difficulties attending the construction of full solutions $P(x, \tau)$ from terms of type (2.9) have been discussed in detail in I (see also Hoare 1971). In the present case we expect them to take the form

$$P(x, \tau) = \pi^{-1/2} e^{-x^2} + e^{-\frac{1}{2}x^2} \sum_k a_k \phi_k(x) e^{-\lambda_k \tau} + e^{-\frac{1}{2}x^2} \int_1^\infty \omega(\lambda)\phi(x, \lambda) e^{-\lambda\tau} d\lambda. \tag{2.12}$$

In this the first term is the equilibrium maxwellian, arising from $\lambda = 0$, the second is the contribution from discrete relaxation modes with $0 < \lambda_k < 1$ in the τ time scale and the third gives the influence of the continuous spectrum—the totality of the interval $(1, \infty)$, where the equation $z(x) - \lambda = 0$ has real roots $x = \pm x_\lambda$. We recall that the reality of all eigenvalues and the positive definiteness of the spectrum is guaranteed by the symmetry of the kernel $g(x, y)$ and the conservation of probability underlying equation (2.2). The expansion coefficients a_k and the function $\omega(\lambda)$ are to be determined by the initial condition $P(x, 0)$; their existence (in the sense that the right-hand side of (2.12) can be made to converge in the mean to the correct $P(x, \tau)$ for all τ) is not a foregone conclusion but requires the *completeness* of the solution set $\{\phi_k(x), \phi(x, \lambda)\}$ with respect to a sufficiently inclusive class of physically interesting probability functions. Since the eigenfunctions $\phi(x, \lambda)$ prove to be *distributions* in the sense of Schwartz, proof of completeness and construction of the expansion function $\omega(\lambda)$ are somewhat complicated.

3. Emptiness of the discretum

A distinguishing feature of the Rayleigh problem for equal masses is that there prove to exist no discrete eigenvalues λ_k in the allowed interval $0 < \lambda_k < 1$. This leaves only the singular eigenfunctions $\phi(x, \lambda)$ as the basis for constructing the transient part of the initial-value solutions.

In order to prove the emptiness of the discretum it is convenient to work not with the symmetric eigenvalue equation (2.10) but with a simpler, unsymmetric form obtained by substituting

$$f(x, \lambda) = e^{\frac{1}{2}x^2}\phi(x, \lambda). \tag{3.1}$$

The integral equation now becomes

$$[z(x) - \lambda]f(x, \lambda) = \int_{-\infty}^{\infty} |x - y| e^{-y^2} f(y, \lambda) dy \tag{3.2}$$

which may then be reduced to a differential equation by use of the symbolic operation $(d^2/dx^2)|x - y| = 2\delta(x - y)$. Thus we find

$$(d^2/dx^2)\{[z(x) - \lambda]f(x, \lambda)\} = 2e^{-x^2} f(x, \lambda). \tag{3.3}$$

The solution of this, which we have already sketched in part I, follows straightforwardly on noting the simple first and second derivatives of the function $z(x)$. Thus, from (2.8), we see that

$$z'(x) = \pi^{1/2} \operatorname{erf}(x) \tag{3.4}$$

$$z''(x) = 2 \exp(-x^2). \tag{3.5}$$

Given the relation (3.5) one solution of (3.3) can be seen immediately to be $f(x, \lambda) = A$, an arbitrary constant. A second, independent solution then emerges as

$$f(x, \lambda) = \int^{x} \frac{\mathrm{d}y}{[z(y)-\lambda]^2}. \tag{3.6}$$

Since for the moment we confine interest to the region $\lambda < 1$, the denominator cannot vanish and the indefinite integral is a proper one. The general solution to (3.3) can thus be written

$$f(x, \lambda) = A + BR(x, \lambda) \tag{3.7}$$

where we have now specified

$$R(x, \lambda) = \int_0^{x} \frac{\mathrm{d}y}{[z(y)-\lambda]^2}. \tag{3.8}$$

It remains to substitute back into the original integral equation (3.2) so as to fix the constants A and B according to the boundary conditions implicit in this and arrive at eigenvalues, if any, in the discretum range $\lambda < 1$. The manipulation involved is not entirely straightforward and we require a number of indefinite integrals, which will also be useful later. In particular we define and evaluate by partial integration the two functions:

$$\begin{aligned} Q_1(x, \lambda) &= \int^{x} \mathrm{e}^{-x^2} R(x, \lambda)\, \mathrm{d}x \\ &= \tfrac{1}{2} R(x, \lambda) z'(x) + \tfrac{1}{2}[z(x)-\lambda]^{-1} \end{aligned} \tag{3.9}$$

and

$$\begin{aligned} Q_2(x, \lambda) &= \int^{x} x\, \mathrm{e}^{-x^2} R(x, \lambda)\, \mathrm{d}x \\ &= \tfrac{1}{2} x[z(x)-\lambda]^{-1} + \tfrac{1}{2}(\lambda - \mathrm{e}^{-x^2}) R(x, \lambda). \end{aligned} \tag{3.10}$$

In proving the second we have used the special relationship

$$z(x) = \mathrm{e}^{-x^2} + x z'(x). \tag{3.11}$$

Taking these results together with the limit

$$\lim_{x \to \pm\infty} \left(\frac{x}{z(x)-\lambda} \right) = \lim_{x \to \pm\infty} \left(\frac{1}{z'(x)} \right) = \pm \pi^{-1/2} \tag{3.12}$$

we arrive at the following condition to be satisfied:

$$\lambda A = B \pi^{1/2} x \int_0^{\infty} \frac{\mathrm{d}y}{[z(y)-\lambda]^2} - \frac{B}{\pi^{1/2}}. \tag{3.13}$$

Because the integral on the right cannot vanish, it follows that the only possible condition for non-singular solution with $\lambda > 0$ is the trivial one $A = B = 0$. Note that, when we allow the special case $\lambda = 0$, the condition changes to A arbitrary, $B = 0$, and we recover the equilibrium solution $f(x, 0) = A$ already determined.

We thus conclude that, with λ in the range $0 < \lambda < 1$, for which the occurrence of eigenvalues is at first conceivable, none actually occur. The discretum is empty.

4. The continuum eigenfunctions

With the discretum empty, the interpretation of the initial-value solution (2.12) turns entirely upon the nature of the continuum eigenfunctions $\phi(x, \lambda)$ with $\lambda \geqslant 1$. These are no longer square integrable on $(-\infty, +\infty)$ and must be considered as generalized functions, singular distributions in the sense of Schwartz. Nevertheless, they can be expected to show an orthogonality property arising from the symmetry of the original integral operator. In the following sections we shall determine the explicit form of the functions $\phi(x, \lambda)$, demonstrate their orthogonality and completeness and obtain the normalization integrals required for the initial-value expansion functions $\omega(\lambda)$.

The general character of the solutions of the singular differential equation (3.3) has already been exposed in the previous section, except that a radical change in the interpretation of $R(x, \lambda)$ is needed for $\lambda \geqslant 1$. The appropriate extension is well known in distribution theory, though we are not aware of any previous occurrence in statistical physics. The 'function' $R(x, \lambda)$ is to be considered as a *pseudofunction* belonging to the class of singular distributions generated by Hadamard's finite part of a generally divergent integral (see Schwartz 1966, chap 2, p 38, Zemanian 1965, §§ 1.4 and 2.5). As such it is undetermined at the points $x = \pm x_\lambda$, but well defined in its action on a given test function $\varphi(x)$. Following the above authors we write

$$\text{Pf. } R(x, \lambda) = \text{Pf.} \int_0^x \frac{\mathrm{d}y}{[z(y) - \lambda]^2} \tag{4.1}$$

with the integral now taken as definite. The functional $\langle R, \varphi \rangle$ arising by action of R is then understood as

$$\langle R, \varphi \rangle = \text{Fp} \int_a^b R(x, \lambda) \varphi(x) \, \mathrm{d}x \tag{4.2}$$

where Fp indicates the taking of a Hadamard finite part whenever the range of integration includes the singularity at $x = x_\lambda$†. A more detailed account of the function $R(x, \lambda)$ and the process of extracting finite parts will be found in the appendix.

4.1. *The singular boundary conditions*

Following the usual requirement for the solution of singular equations (see eg Cercignani 1969) we are forced to augment the solution $f(x, \lambda)$ with a delta function at the singularity.

† We follow Zemanian (1965) in distinguishing between the actual pseudofunction (Pf.) and the finite part arising in a given application of it under an integral (Fp). Schwartz uses the Pf. notation in both cases. In the following we shall drop the prefixes in detailed mathematics whenever it is clear from the context that singular integrals are involved.

Thus the correct form of $f(x, \lambda)$ over the whole range of x and λ is

$$f(x, \lambda) = A(\lambda) + B(\lambda)\delta[z(x) - \lambda] + C(\lambda)\mathrm{Pf.}\, R(x, \lambda) \tag{4.3}$$

where A, B and C are as yet undetermined functions of λ over the region $\lambda > 1$.

The problem of fitting the three arbitrary functions to the boundary conditions implicit in the integral equation (3.2) remains one of considerable complexity. Recalling the root condition $z(\pm x_\lambda) - \lambda = 0$, it will be convenient to divide the x axis into three regions, which we shall designate as follows

$$\begin{aligned} \mathscr{R}_1: &\quad -\infty < x \leqslant -x_\lambda \\ \mathscr{R}_2: &\quad -x_\lambda < x < x_\lambda \\ \mathscr{R}_3: &\quad x_\lambda < x < \infty, \end{aligned}$$

such that the singularities occur only at the two boundaries. Recognizing that the solution of equation (2.10) may well require different values of the constants for each region we assume the form

$$f(x, \lambda) = \begin{cases} A_1(\lambda) + B_1(\lambda)\delta[z(x) - \lambda] + C_1(\lambda)R(x, \lambda) : \mathscr{R}_1 \\ A_2(\lambda) + C_2(\lambda)R(x, \lambda) \qquad\qquad\qquad : \mathscr{R}_2 \\ A_3(\lambda) + B_3(\lambda)\delta[z(x) - \lambda] + C_3(\lambda)R(x, \lambda) : \mathscr{R}_3 . \end{cases} \tag{4.4}$$

Here we have made the only obvious simplification, omitting the delta function from the region $\mathscr{R}_2$.

We must now carry out the tedious process of substituting each of the above alternatives back into the original integral equation. Since the three regions require broadly similar manipulations, only the process for the region $\mathscr{R}_1$ will be described in any detail.

4.2. *The region* $\mathscr{R}_1$

Substituting the solution (4.4) into the integral equation (3.2) the action of the integral operator on the right becomes

$$\begin{aligned} &\int_{-\infty}^{+\infty} |x-y|\, \mathrm{e}^{-y^2} f(y, \lambda)\, \mathrm{d}y \\ &\quad = \int_{-\infty}^{-x_\lambda} |x-y|\, \mathrm{e}^{-y^2} f_1(y, \lambda)\, \mathrm{d}y \qquad (T_1) \\ &\quad + \int_{-x_\lambda}^{x_\lambda} |x-y|\, \mathrm{e}^{-y^2} f_2(y, \lambda)\, \mathrm{d}y \qquad (T_2) \\ &\quad + \int_{x_\lambda}^{\infty} |x-y|\, \mathrm{e}^{-y^2} f_3(y, \lambda)\, \mathrm{d}y \qquad (T_3) \end{aligned} \tag{4.5}$$

where the functions f_1, f_2 and f_3 represent the alternatives for $f(x, \lambda)$ in the three regions according to (4.4). Consider now the integral labelled T_1 above. This splits into some eight further integrals as follows:

$$\int_{-\infty}^{-x_\lambda} |x-y|\, e^{-y^2} f_1(y,\lambda)\, dy$$

$$= \int_{-\infty}^{x} (x-y) f_1(y,\lambda)\, dy + \int_{x}^{x_\lambda} (y-x) f_1(y,\lambda)\, dy$$

$$= A_1\left[x\left(\int_{-\infty}^{x} e^{-y^2}\, dy - \int_{x}^{-x_\lambda} e^{-y^2}\, dy\right) + \int_{x}^{-x_\lambda} y\, e^{-y^2}\, dy - \int_{-\infty}^{x} y\, e^{-y^2}\, dy\right]$$

$$+ B_1\left[\int_{-\infty}^{x} (x-y)\, e^{-y^2}\, \delta[z(y)-\lambda]\, dy + \int_{x}^{-x_\lambda} (y-x)\, e^{-y^2}\, \delta[z(y)-\lambda]\, dy\right]$$

$$+ C_1\left[\int_{-\infty}^{x} (x-y)\, e^{-y^2} R(y,\lambda)\, dy + \int_{x}^{-x_\lambda} (y-x)\, e^{-y^2} R(y,\lambda)\, dy\right] \qquad (4.6)$$

with the taking of finite parts implied in the last term. Of these terms, that multiplying C_1 proves to be the most crucial. The integrals in the second part involve generalizations of the quantities $Q_1(x, \lambda)$ and $Q_2(x, \lambda)$ in the limit where the singularity moves to the end point. Modifying the results (3.9) and (3.10) to read

$$\mathrm{Pf.}\, Q_1(x,\lambda) = \tfrac{1}{2}\mathrm{Pf.}\, R(x,\lambda) z'(x) + \tfrac{1}{2}\mathrm{Pv}\ [z(x)-\lambda]^{-1} \qquad (4.7)$$

and

$$\mathrm{Pf.}\, Q_2(x,\lambda) = \tfrac{1}{2} x \mathrm{Pv}\ [z(x)-\lambda]^{-1} + \tfrac{1}{2}\mathrm{Pf.}\, (\lambda - e^{-x^2}) R(x,\lambda) \qquad (4.8)$$

(note that the Cauchy principal value Pv can replace the Fp prescription when the singularity is logarithmic and not at an end point), we see that the integrals in question are undoubtedly divergent in the limits $Q_1(x_\lambda, \lambda)$, $Q_2(x_\lambda, \lambda)$. Before drawing conclusions from this, however, we still need the results of substitution in all three regions. Still working in $\mathscr{R}_1$ the group of integrals $A_1[\quad]$ may be considered. A series of elementary integrations reduces this to

$$A_1[\quad] \equiv A_1[z(x) + \tfrac{1}{2}x(\pi^{1/2} + z'(x_\lambda) - \tfrac{1}{2}\, e^{-x_\lambda^2})]. \qquad (4.9)$$

Lastly, the delta function terms with coefficient B_1 yield

$$B_1[\quad]\begin{cases} \equiv -\tfrac{1}{4}B_1(x+x_\lambda)\, e^{-x_\lambda^2}/z'(x_\lambda); & x < x_\lambda \\ = 0; & x = x_\lambda. \end{cases} \qquad (4.10)$$

Here we have used the prescription (Jones 1966, p 150)

$$\int_a^b f(x)\delta(x-b)\, dx = \tfrac{1}{2} f(b). \qquad (4.11)$$

Other properties of the delta function which we shall need constantly are the relation

$$\int_a^b f(x)\delta[g(x)-g(c)]\, dx = |g'(c)|^{-1} f(c) \qquad (a < c < b) \qquad (4.12)$$

and the convolution

$$\delta(x) * \delta(y) = \int_a^b \delta(x-w)\delta(w-y)\, dw = \delta(x-y). \qquad (4.13)$$

Addition of these results completes the evaluation of the term T_1 in equation (4.5). It is now necessary to carry out similar reductions for the integrals T_2 and T_3 before the test of the solution in $\mathscr{R}_1$ is complete. The whole procedure is then repeated in broadly similar fashion for the regions $\mathscr{R}_2$ and $\mathscr{R}_3$. When finally composed from these results, the condition for solution in $\mathscr{R}_1$ takes the form

$$\begin{aligned} -\lambda A_1 = {} & \{\tfrac{1}{2}(A_3-A_1)\,\mathrm{e}^{-x_\lambda^2}+\tfrac{1}{2}(B_3-B_1)x_\lambda\,\mathrm{e}^{-x_\lambda^2}/z'(x_\lambda)-C_1(\tfrac{1}{2}\pi^{-1/2}+\tfrac{1}{2}\lambda R(\infty,\lambda)+Q_2(x_\lambda)) \\ & +2C_2Q_2(x_\lambda)+C_3(\tfrac{1}{2}\pi^{-1/2}+\tfrac{1}{2}\lambda R(\infty,\lambda)-Q_2(x_\lambda))\} \\ & +x[\tfrac{1}{2}\pi^{1/2}(A_1-A_3)+\tfrac{1}{2}z'(x_\lambda)(A_1-2A_2+A_3)-\tfrac{1}{2}(B_1+B_3)\,\mathrm{e}^{-x_\lambda^2}/z'(x_\lambda) \\ & +(C_3-C_1)Q_1(x_\lambda)-\tfrac{1}{2}(C_1+C_3)\pi^{1/2}R(\infty,\lambda)]. \end{aligned} \tag{4.14}$$

In the above equation, factors of $z(x)$ have already been cancelled, leaving it only necessary to force solution by the two conditions

$$[\quad]=0, \qquad \{\quad\}+\lambda A_1=0.$$

4.3. *The full range*

A pair of equations of this type is obtained for each region making in all six equations in eight unknowns. The remaining information will prove to be contained in an analyticity condtion and a normalization. The six explicit conditions take the following form (note that $R(\infty, \boldsymbol{n})$ is here an *ordinary* function of $\boldsymbol{n}$ the taking of the necessary finite part being implied) (from $\mathscr{R}_1$):

$$\begin{aligned} & \tfrac{1}{2}\pi^{1/2}(A_1-A_3)+\tfrac{1}{2}(A_1-2A_2+A_3)z'(x_\lambda)-\tfrac{1}{2}(B_1+B_3)\,\mathrm{e}^{-x_\lambda^2}/z'(x_\lambda)-(C_1-C_3)Q_1(x_\lambda) \\ & \qquad -\tfrac{1}{2}\pi^{1/2}(C_1+C_3)R(\infty,\lambda)=0. \end{aligned} \tag{4.15}$$

$$\begin{aligned} & \tfrac{1}{2}(A_3-A_1)\,\mathrm{e}^{-x_\lambda^2}+\tfrac{1}{2}(B_3-B_1)x_\lambda\,\mathrm{e}^{-x_\lambda^2}/z'(x_\lambda)-\tfrac{1}{2}(C_1-C_3)(\pi^{-1/2}+\lambda R(\infty,\lambda)) \\ & \qquad -(C_1-2C_2+C_3)Q_2(x_\lambda)+\lambda A_1=0. \end{aligned} \tag{4.16}$$

(from $\mathscr{R}_2$):

$$\begin{aligned} & \tfrac{1}{2}(A_1-A_3)(\pi^{1/2}-z'(x_\lambda))+\tfrac{1}{2}(B_1-B_3)\,\mathrm{e}^{-x_\lambda^2}/z'(x_\lambda)+(C_1+C_3)(Q_1(x_\lambda)-\tfrac{1}{2}\pi^{1/2}R(\infty,\lambda)) \\ & \qquad -2C_2Q_1(x_\lambda)=0 \end{aligned}$$

$$\begin{aligned} & \tfrac{1}{2}(A_1-2A_2+A_3)\,\mathrm{e}^{-x_\lambda^2}+\tfrac{1}{2}(B_1+B_3)x_\lambda\,\mathrm{e}^{-x_\lambda^2}/z'(x_\lambda)-\tfrac{1}{2}(C_1-C_3)(\pi^{-1/2}+\lambda R(\infty,\lambda) \\ & \qquad -2Q_2(x_\lambda))+\lambda A_2=0 \end{aligned} \tag{4.17}$$

(from $\mathscr{R}_3$):

$$\begin{aligned} & \tfrac{1}{2}\pi^{1/2}(A_1-A_3)-\tfrac{1}{2}(A_1-2A_2+A_3)z'(x_\lambda)+\tfrac{1}{2}(B_1+B_3)\,\mathrm{e}^{-x_\lambda^2}/z'(x_\lambda)+(C_1-C_3)Q_1(x_\lambda) \\ & \qquad -\tfrac{1}{2}\pi^{1/2}(C_1+C_3)R(\infty,\lambda)=0 \end{aligned} \tag{4.18}$$

$$\begin{aligned} & \tfrac{1}{2}(A_1-A_3)\,\mathrm{e}^{-x_\lambda^2}+\tfrac{1}{2}(B_1-B_3)x_\lambda\,\mathrm{e}^{-x_\lambda^2}/z'(x_\lambda)+\tfrac{1}{2}(C_1-C_3)(\pi^{-1/2}+\lambda R(\infty,\lambda)) \\ & \qquad +(C_1-2C_2+C_3)Q_2(x_\lambda)+\lambda A_3=0. \end{aligned} \tag{4.19}$$

We first make use of the analyticity condition. Since both $Q_1(x_\lambda)$ and $Q_2(x_\lambda)$ are known to be singular, it follows that the coefficients of these terms must vanish. Thus each of the three sets of equations consistently require

$$C_1 = C_2 = C_3. \tag{4.20}$$

Simple algebra then leads to the following connections:

$$B_1 = (A_1 - A_2)\, e^{x_\lambda^2}[z'(x_\lambda)]^2 \tag{4.21}$$

$$B_3 = (A_1 + A_2)\, e^{x_\lambda^2}[z'(x_\lambda)]^2 \tag{4.22}$$

$$A_3 = -A_1 \tag{4.23}$$

$$C_1 = C_2 = C_3 = A_1/R(\infty, \lambda). \tag{4.24}$$

We have thus been able to reduce the form of the solution to one containing only two arbitrary constants A_1 and A_2. Finally, reverting to the original eigenfunctions $\phi(x, \lambda)$ we obtain

$$\phi(x,\lambda) = A_1\, e^{-\frac{1}{2}x^2} R(x,\lambda)/R(\infty,\lambda) + e^{-\frac{1}{2}x^2} \begin{cases} A_1 + (A_1 - A_2)\, e^{x_\lambda^2} z'(x_\lambda)^2 \delta[z(x) - \lambda]; & x \leqslant -x_\lambda \\ A_2; & |x| < x_\lambda \\ -A_1 - (A_1 - A_2)\, e^{x_\lambda^2} z'(x_\lambda)^2 \delta[z(x) - \lambda]; & x \geqslant x_\lambda. \end{cases} \tag{4.25}$$

Having thus solved the eigenvalue problem for the singular operator $\mathscr{H}$, considerable work remains before we can exploit the eigenfunctions in an expansion of the initial-value solution such as (2.12). In particular we must prove orthogonality and completeness and determine the normalization function. These questions, all of them problematic in view of the singular nature of the distributions involved, will be taken up in §§ 5, 6 and 7.

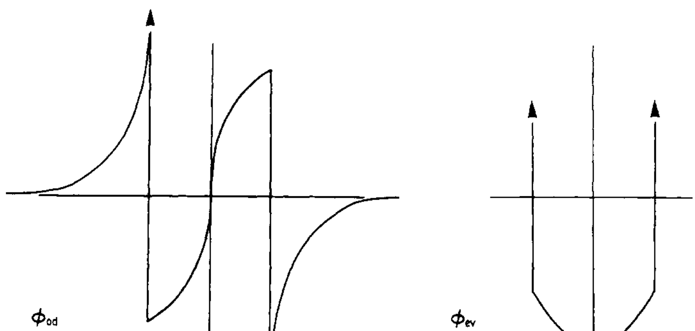

Figure 2. Singular eigenfunctions of the Rayleigh piston ($\gamma = 1$). Left: odd functions ϕ_{od}. Right: even functions ϕ_{ev}. The delta function components occurring at $x = \pm x_\lambda$ are indicated by arrowheads (schematic only) (equations (5.1), (5.2)).

5. Symmetry properties: the half-range problem

A number of symmetry properties emerge at this stage. We notice first that the eigenfunction solution just found divides naturally into odd and even components, which are simply the terms carrying the coefficients A_1 and A_2 respectively. Thus it is convenient to write

$$\phi(x, \lambda) = A_1\phi_{\mathrm{od}}(x, \lambda) + A_2\phi_{\mathrm{ev}}(x, \lambda)$$

where

$$\phi_{\mathrm{od}}(x, \lambda) = \mathrm{e}^{-\frac{1}{4}x^2}R(x, \lambda)/R(\infty, \lambda)$$
$$\begin{cases} -\mathrm{e}^{-\frac{1}{4}x^2}(\operatorname{sgn} x)[1+\mathrm{e}^{x_\lambda^2}z'(x_\lambda)^2\delta[z(x)-\lambda]]; & |x| \geqslant x_\lambda \\ +0; & |x| < x_\lambda \end{cases} \tag{5.1}$$

$$\phi_{\mathrm{ev}}(x, \lambda) = \begin{cases} -\mathrm{e}^{-\frac{1}{4}x^2+x_\lambda^2}z'(x_\lambda)^2\delta[z(x)-\lambda]; & |x| \geqslant x_\lambda \\ +\mathrm{e}^{-\frac{1}{4}x^2}; & |x| < x_\lambda. \end{cases} \tag{5.2}$$

The general appearance of the odd and even eigenfunctions is illustrated in figure 2.

The property underlying this simplification is, of course, the symmetry of the scattering kernel with respect to *inverse* collisions

$$g(-x, y) = g(x, -y) \tag{5.3}$$

which holds in addition to the *reverse* collision symmetry, $g(x, y) = g(y, x)$, giving detailed balance and reality of λ.

The symmetry (5.3) has two essential consequences. First, the odd and even components of the solution $\phi(x, \lambda)$ must separately be eigenfunctions of the singular operator $\mathscr{H}$ (equation (2.11)). To see this we symmetrize both sides of the integral equation (2.10) and apply (5.3) to give

$$[z(x)-\lambda]\phi_{\mathrm{ev}}(x) = \tfrac{1}{2}\int_{-\infty}^{+\infty}[g(x, y)+g(x, -y)]\phi(y)\,\mathrm{d}y. \tag{5.4}$$

Because the combined kernel on the right is now even in y, the odd component in ϕ is annihilated and the two terms in the integral contribute identically. Thus it follows that $\mathscr{H}\phi_{\mathrm{ev}} = \lambda\phi_{\mathrm{ev}}$ and automatically also that $\mathscr{H}\phi_{\mathrm{od}} = \lambda\phi_{\mathrm{od}}$.

A more physical elucidation of (5.3) is that, if we define a *speed* kernel, $\hat{g}(x, y)$, by summing over the four combinations of directions:

$$\hat{g}(x, y) = g(x, y)+g(x, -y)+g(-x, y)+g(-x, -y)$$

then the set $\{\phi_{\mathrm{ev}}\}$ alone are eigenfunctions of the corresponding half-range operator $\hat{\mathscr{H}}$ which governs the relaxation problem for the probability distribution $P(|V|, t)$. The explicit form of the kernel for the half-range operator is easily shown to be

$$\hat{H}(x, y) = z(x)\delta(x-y) - 2\max(x, y)\exp[-\tfrac{1}{2}(x^2+y^2)] \tag{5.5}$$

this arising in turn by symmetrization and scaling of the actual speed-transition kernel:

$$\hat{K}(|V|, |V'|) = 4n\sigma\max(|V|, |V'|)f_M(V'). \tag{5.6}$$

The solution of the speed-initial-value problem is then somewhat simpler than equation (2.12) implies, namely

$$P(|x|, \tau) = 2\pi^{1/2}\,e^{-x^2} + e^{-\frac{1}{2}x^2}\int_1^\infty \omega_1(\lambda)\phi_{ev}(x, \lambda)\,e^{-\lambda\tau}\,d\lambda. \tag{5.7}$$

The validity of this expression still depends, however, on our ability to demonstrate the half-range completeness of the set $\{\phi_{ev}\}$ for a sufficient class of initial conditions $P(|x|, 0)$. This question is taken up in § 7. We first need to establish the orthogonality of the eigenfunctions within the two symmetry subsets.

6. Orthogonality properties

Although the symmetry of the original integral equation leads us to believe that the eigenfunctions $\phi(x, \lambda)$ form a mutually orthogonal set, their singular character makes it advisable to check that the relevant integrals do indeed vanish as expected. Assuming that orthogonality can be demonstrated, we shall require in addition the normalization function $N(\lambda)$ giving the λ dependence of the inner product of each eigenfunction with itself. It will be shown that the latter quantity, though also singular, is well defined by virtue of the convolution property of the delta functions. Several cases occur.

(*a*) *General orthogonality of* $\phi(x, \lambda)$

From the general symmetry properties we have, for the full range:

$$(\phi_{od}(\lambda), \phi_{ev}(\lambda)) = 0, \qquad (-\infty < x < \infty),$$

from which it follows that the inner products of ϕ, ϕ_{od} and ϕ_{ev} are related through

$$(\phi(\lambda), \phi(\lambda')) = A_1^2(\phi_{od}(\lambda), \phi_{od}(\lambda')) + A_2^2(\phi_{ev}(\lambda), \phi_{ev}(\lambda')). \tag{6.1}$$

Thus the separate symmetry types may be considered independently.

(*b*) *Orthogonality of* $\phi(x, \lambda)$ *to the maxwellian*

The simplest case to prove is the orthogonality of the equilibrium eigenfunction $\phi_0(x)$ to the whole set $\phi(x, \lambda)$ with $1 < \lambda < \infty$. To show that $(\phi_0, \phi(\lambda)) = 0$ for the full range, it clearly suffices to verify that

$$\int_0^\infty e^{-\frac{1}{2}x^2}\phi_{ev}(x, \lambda)\,dx = 0, \qquad (1 < \lambda < \infty). \tag{6.2}$$

Writing the singular part of ϕ_{ev} explicitly, we see that

$$(\phi_0, \phi(\lambda)) = \text{constant} \times \left(\int_0^{x_\lambda} e^{-x^2}\,dx - \int_{x_\lambda}^\infty [z'(x)]^2\delta[z(x)-\lambda]\,dx\right).$$

Using now the relations (3.4), (4.9) and (4.10) it is found that both the integrals equal $\frac{1}{2}\pi^{1/2}\,\mathrm{erf}(x_\lambda)$ and cancel. Thus, as expected

$$(\phi_0, \phi(\lambda)) = (\phi_0, \phi_{od}(\lambda)) = (\phi_0, \phi_{ev}(\lambda)) = 0 \qquad \text{(full range)} \tag{6.3}$$

and

$$(\phi_0, \phi_{ev}(\lambda)) = 0 \qquad \text{(half range)}. \tag{6.4}$$

(c) Orthogonality among $\{\phi_{\text{od}}\}$ *and* $\{\phi_{\text{ev}}\}$

It is somewhat more difficult to prove that the sets $\{\phi_{\text{od}}\}$ and $\{\phi_{\text{ev}}\}$ are orthogonal within themselves for all values of $\lambda > 1$, ie that

$$\int_{-\infty}^{\infty} \phi(x, \lambda)\phi(x, \lambda')\,\mathrm{d}x = N(\lambda)\delta(\lambda-\lambda'). \tag{6.5}$$

There appears to be no great advantage in treating the symmetry types separately, and we have not been able to improve on the direct approach of splitting the integral into five ranges and examining each:

$$(\phi(\lambda), \phi(\lambda')) = \int_{-\infty}^{+\infty} \phi(x, \lambda)\phi(x, \lambda')\,\mathrm{d}x = \int_{-\infty}^{-x_\lambda} + \int_{-x_\lambda}^{-x_{\lambda'}} + \int_{-x_{\lambda'}}^{x_{\lambda'}} + \int_{x_{\lambda'}}^{x_\lambda} + \int_{x_\lambda}^{\infty}.$$

Here we have assumed $\lambda' \leqslant \lambda$ so that correspondingly $x_{\lambda'} \leqslant x_\lambda$.

The detailed examination of the five integrals proves somewhat tedious and the symmetry properties are only of slight help. The indefinite singular integrals $Q_1(x, \lambda)$ and $Q_2(x, \lambda)$ (equations (3.9) and (3.10), (4.7) and (4.8)) are required together with the related result

$$\text{Pf. } Q_3(x, \lambda, \lambda') = \text{Pf.} \int^{x} \mathrm{e}^{-x^2} R(x, \lambda)R(x, \lambda')\,\mathrm{d}x$$

$$= z'(x)R(x, \lambda)R(x, \lambda') + \frac{R(x, \lambda)}{z(x)-\lambda'} + \frac{R(x, \lambda')}{z(x)-\lambda} + \frac{1}{\lambda-\lambda'}[R(x, \lambda)-R(x, \lambda')] \tag{6.6}$$

(with the prefix Pf. implied as necessary). At each stage care is needed particularly in keeping account of the delta functions which arise from integrals with singularity at an end point (see the appendix). However, both these and the logarithmic singularities arising from (6.6) above cancel correctly, leaving only the essential delta function arising from the convolution $\delta[z(x)-\lambda]*\delta[z(x)-\lambda']$.

The final result is

$$(\phi(\lambda), \phi(\lambda')) = (A_1^2 + A_2^2)[z'(x_\lambda)]^3\,\mathrm{e}^{+x_\lambda^2}\delta(\lambda-\lambda'). \tag{6.7}$$

The constants A_1 and A_2 being arbitrary, we can equally well write the conditions

$$(\phi_{\text{od}}(\lambda), \phi_{\text{ev}}(\lambda')) = (\phi_{\text{ev}}(\lambda), \phi_{\text{ev}}(\lambda')) = \nu(\lambda)\delta(\lambda-\lambda') \tag{6.8}$$

with

$$\nu(\lambda) = [z'(x_\lambda)]^3\,\mathrm{e}^{+x_\lambda^2}. \tag{6.9}$$

Various choices are now open for the normalization of the different sets. We shall take the odd and even subsets to satisfy (6.8) unchanged and leave the arbitrariness in the combinations, writing for the overall normalization function

$$N(\lambda) = (A_1^2 + A_2^2)\nu(\lambda). \tag{6.10}$$

The persistence of two constants in the final result is no problem, being simply an indication that the odd and even components of any function to be represented must appear separately throughout, in a way reminiscent of elementary Fourier analysis.

6.1. Odd–even symmetry and the initial-value problem

The separability of the eigenfunctions into odd and even subsets has important consequences for the expression of the time-dependent distribution function $P(x, \tau)$. Noting that the eigenfunctions $\phi(x, \lambda)$ can equally well be considered as functions $\phi(x, x_\lambda)$, and that $d\lambda = z'(x_\lambda)\, dx_\lambda$, the integral in equation (5.7) can clearly be transformed to one over the variable x_λ with the transient factor $\exp[-z(x_\lambda)\tau]$. Furthermore, since examination of the explicit forms shows that the functions $\phi(x, x_\lambda)$ are undoubtedly even in x_λ, it follows that $\omega(x_\lambda)$ may also be taken as even, because any odd component would be annihilated in the integral. Thus the lower limit can be changed to zero and the modified initial-value solution written

$$P(x, \tau) = \pi^{-1/2}\, e^{-x^2} + e^{-\frac{1}{2}x^2} \int_0^\infty \omega(x_\lambda) z'(x_\lambda) \phi(x, x_\lambda)\, e^{-z(x_\lambda)\tau}\, dx_\lambda. \qquad (6.11)$$

The expansion function $\omega(x_\lambda)$ is now to be fitted by the initial distribution

$$P(x, 0) = \pi^{-1/2}\, e^{-x^2} + e^{-\frac{1}{2}x^2} \int_0^\infty \omega(x_\lambda) z'(x_\lambda) \phi(x, x_\lambda)\, dx_\lambda. \qquad (6.12)$$

In the next section we shall detail a constructive proof of the completeness of the set of eigenfunctions $\phi(x, x_\lambda)$ for a satisfactory class, ie one which both demonstrates the existence of an expansion function $\omega(x_\lambda)$ satisfying (6.12) in the mean and provides a method for obtaining it.

7. Proof of full- and half-range completeness

The set $\{\phi(x, \lambda)\}$ being defined in terms of a continuous parameter, we may anticipate that the representation (6.11), if it exists, will be somewhat in the nature of a Fourier integral. For our purposes completeness is only required with respect to a satisfactory class of probability functions $P(x, 0)$ and proof of it will consist in demonstrating that a solution $\omega(\lambda)$ always exists such as to make equation (6.11) valid for this class†.

Since the odd and even subsets of the basis separate naturally and moreover have a distinct physical interpretation, it will be convenient to treat the completeness of each symmetry type separately with respect to probability functions of the same parity. This we can do by making the decomposition

$$P(x, 0) = P_{ev}(x, 0) + P_{od}(x, 0) \qquad (7.1)$$

where

$$P_{ev}(x, 0) = \tfrac{1}{2}[P(x, 0) + P(-x, 0)] \qquad (7.2)$$

and

$$P_{od}(x, 0) = \tfrac{1}{2}[P(x, 0) - P(-x, 0)]. \qquad (7.3)$$

† Validity here implies convergence in the mean for the right-hand side as an upper limit in the integral tends to infinity. Experience in transport theory shows that, with singular basis sets, it is not usually possible to specify precisely the class of functions for which completeness is guaranteed. This class will, however, usually be more comprehensive than that of the L_2 functions and must be required to include certain distributions such as $\delta(x - x_0)$. A common, though rather casual, procedure is to require completeness with respect to a class of 'reasonable' functions, defined as those whose modulus possesses a Laplace transform.

Using the eigenfunctions according to equations (5.1) and (5.2), we then have two separate expansion problems

$$P_{\mathrm{ev}}(x,0) = \pi^{-1/2}\,\mathrm{e}^{-x^2} + \mathrm{e}^{-\frac{1}{2}x^2}\int_0^\infty \omega_1(x_\lambda)\phi_{\mathrm{ev}}(x,x_\lambda)z'(x_\lambda)\,\mathrm{d}x_\lambda \tag{7.4}$$

and

$$P_{\mathrm{od}}(x,0) = \mathrm{e}^{-\frac{1}{2}x^2}\int_0^\infty \omega_2(x_\lambda)\phi_{\mathrm{od}}(x,x_\lambda)z'(x_\lambda)\,\mathrm{d}x_\lambda. \tag{7.5}$$

The two expansion functions are designated ω_1 and ω_2, both being, as we have seen, even functions. Note that the inclusion of the maxwellian in the even expansion means that we are concerned, in effect, only with the component orthogonal to this.

7.1. Even completeness

The completeness of the functions $\phi_{\mathrm{ev}}(x,\lambda)$ is relatively easy to settle. Interpreting the delta functions in the expressions (5.2), the right-hand side of (7.4) reduces so that

$$P_{\mathrm{ev}}(x,0) = \pi^{-1/2}\,\mathrm{e}^{-x^2} + \tfrac{1}{2}\omega_1(x)[z'(x)]^2 - \mathrm{e}^{-x^2}\int_{|x|}^\infty z'(x_\lambda)\omega_1(x_\lambda)\,\mathrm{d}x_\lambda. \tag{7.6}$$

Multiplying this equation by $\exp(x^2)$, differentiating and then using an obvious integrating factor, we obtain the indefinite integral form below, with β a constant of integration:

$$\omega_1(x) = \frac{1}{[z'(|x|)]^3}\left(2P_{\mathrm{ev}}(x,0)z'(|x|) + \beta\mathrm{e}^{-x^2} - 4\mathrm{e}^{-x^2}\int^x \mathrm{sgn}(y)P_{\mathrm{ev}}(y,0)\,\mathrm{d}y\right). \tag{7.7}$$

Using this back in (7.6), this constant is then found to be

$$\beta = 4\int^\infty \mathrm{sgn}(x)P_{\mathrm{ev}}(x,0)\,\mathrm{d}x \tag{7.8}$$

and the final expression for $\omega_1(x)$ becomes

$$\omega_1(x) = \frac{1}{[z'(|x|)]^3}\left(2P_{\mathrm{ev}}(x,0)z'(|x|) + 4\mathrm{e}^{-x^2}\int_x^\infty \mathrm{sgn}(y)P_{\mathrm{ev}}(y,0)\,\mathrm{d}y\right). \tag{7.9}$$

The required solution for $\omega_1(x)$ clearly exists and can be determined, given only the relatively weak condition that the above integral is finite.

7.2. Odd completeness

The completeness condition to be determined through equation (7.5) proves more troublesome. Entering the solutions (5.1) into the right-hand side we find

$$P_{\mathrm{od}}(x,0) = -\tfrac{1}{2}[z'(x)]^2(\mathrm{sgn}\,x)R(\infty,|x|)\Omega_2(x) - \mathrm{e}^{-x^2}(\mathrm{sgn}\,x)\int_0^{|x|}\Omega_2(y)R(\infty,y)z'(y)\,\mathrm{d}y$$
$$+\mathrm{e}^{-x^2}\int_0^\infty \Omega_2(y)R(x,y)z'(y)\,\mathrm{d}y \tag{7.10}$$

in which we have written

$$\Omega_2(x_\lambda) = \omega_2(x_\lambda)/R(\infty, x_\lambda). \tag{7.11}$$

Noticing that

$$\frac{1}{2}\frac{d}{dx}\left(z'(|x|)\int_0^{|x|}\Omega_2(y)R(\infty, y)z'(y)\,dy\right)$$
$$= \tfrac{1}{2}z'(|x|)^2(\operatorname{sgn} x)\Omega_2(|x|)R(\infty, |x|) + e^{-x^2}(\operatorname{sgn} x)\int_0^{|x|}\Omega_2(y)R(\infty, y)z'(y)\,dy, \tag{7.12}$$

equation (7.10) may be integrated to give

$$\int_{-\infty}^{x} P_{od}(x, 0)\,dx$$
$$= -\tfrac{1}{2}z'(|x|)\int_0^{|x|}\Omega_2(y)R(\infty, y)z'(y)\,dy + \tfrac{1}{2}\pi^{1/2}\int_0^{\infty}\Omega_2(y)R(\infty, y)z'(y)\,dy$$
$$+ \int_{-\infty}^{x} dy\int_0^{\infty}\Omega_2(x_\lambda)z'(x_\lambda)\,e^{-y^2}R(y, x_\lambda)\,dx_\lambda. \tag{7.13}$$

Now, using the particular form of the integral (4.7):

$$\text{Pf.}\int_{-\infty}^{x} e^{-y^2}R(y, x_\lambda)\,dy = \tfrac{1}{2}\{z'(x)R(x, x_\lambda) + \text{Pv}[z(x) - z(x_\lambda)]^{-1} + \pi^{1/2}R(\infty, x_\lambda)\} \tag{7.14}$$

and assuming, reasonably, that the required principal values exist, we may invert the order of integration in the last integral of the previous expression and write for this

$$\int_{-\infty}^{x} dy\int_0^{\infty}\Omega_2(x_\lambda)z'(x_\lambda)\,e^{-y^2}R(y, x_\lambda)\,dx_\lambda$$
$$= \tfrac{1}{2}z'(x)\int_0^{\infty}\Omega_2(x_\lambda)R(x, x_\lambda)z'(x_\lambda)\,dx_\lambda - \tfrac{1}{2}\pi^{1/2}\int_0^{\infty}\Omega_2(x_\lambda)R(\infty, x_\lambda)z'(x_\lambda)\,dx_\lambda$$
$$+ \tfrac{1}{2}\text{Pv}\int_0^{\infty}\frac{\Omega_2(x_\lambda)z'(x_\lambda)\,dx_\lambda}{z(x) - z(x_\lambda)}. \tag{7.15}$$

On substituting back into (7.13) the following singular integral equation for the function Ω_2 is then obtained:

$$\tfrac{1}{4}\,e^{x^2}(z'(x))^3(\operatorname{sgn} x)R(\infty, x)\Omega_2(x) - \tfrac{1}{2}\text{Pv}\int_0^{\infty}\frac{\Omega_2(x_\lambda)z'(x_\lambda)\,dx_\lambda}{z(x) - z(x_\lambda)}$$
$$= \int_{-\infty}^{x} P_{od}(y, 0)\,dy - \tfrac{1}{2}z'(x)\,e^{x^2}P_{od}(x, 0). \tag{7.16}$$

A set of simple transformations puts this into standard notation. We write

$$z(x_\lambda) = \lambda; \qquad z(x) = \lambda_0 \tag{7.17}$$

$$\alpha(\lambda_0) = \tfrac{1}{2}\,e^{x^2}[z'(|x|)]^3R(\infty, x) \tag{7.18}$$

$$g(\lambda_0) = 2\int_{-\infty}^{x} P_{\mathrm{od}}(y, 0)\,\mathrm{d}y - z'(x)\,\mathrm{e}^{x^2} P_{\mathrm{od}}(x, 0) \qquad (7.19)$$

and understand the correspondence $\Omega_2(x) \to \Omega_2(\lambda_0)$ through equation (7.17). The equation above is thereby reduced to

$$\alpha(\lambda_0)\Omega_2(\lambda_0) + \mathrm{Pv}\int_1^\infty \frac{\Omega_2(\lambda)\,\mathrm{d}\lambda}{\lambda-\lambda_0} = g(\lambda_0). \qquad (7.20)$$

This is a singular integral equation of Carleman type, familiar in transport theory. An elementary account will be found in Tricomi (1957); a more rigorous treatment is given by Muskhelishvili (1953). The Carleman equation can be shown by standard methods to have a solution expressible in the form

$$\Omega_2(\lambda_0) = \frac{\alpha(\lambda_0)g(\lambda_0)}{\alpha^2(\lambda_0)+\pi^2} + \frac{\mathrm{e}^{\Gamma(\lambda_0)}}{[\alpha^2(\lambda_0)+\pi^2]^{1/2}}\mathrm{Pv}\int_1^\infty \frac{\mathrm{e}^{-\Gamma(\lambda)}}{[\alpha^2(\lambda)+\pi^2]^{1/2}}\frac{g(\lambda)\,\mathrm{d}\lambda}{\lambda-\lambda_0} \qquad (7.21)$$

with

$$\Gamma(\lambda_0) = \pi^{-1/2}\mathrm{Pv}\int_1^\infty \frac{\theta(\lambda)\,\mathrm{d}\lambda}{\lambda-\lambda_0} \qquad (7.22)$$

the Hilbert transform of the function

$$\theta(\lambda) = \tan^{-1}_{(0,\pi)} \frac{\pi}{\alpha(\lambda)}. \qquad (7.23)$$

A number of mild conditions must be satisfied in order that the solution just written should be uniquely valid. Of these the most important is that $P_{\mathrm{od}}(x, 0)$ be of such a form that the function $g(x)$ defined in (7.19) satisfy a Hölder condition. This will certainly be the case for all 'reasonable' initial probability distributions†. We refer to Wu (1966) for further background on singular equations in kinetic theory and to Guernsey (1960) for detailed discussion on the conditions for uniqueness of solution.

Although the relations just written would present severe computational difficulties, they nevertheless establish the desired result, namely that an expansion function $\omega_2(\lambda)$ exists and can be found under quite acceptable conditions on the odd part of the probability distribution $P(x, 0)$. Moreover, these conditions certainly admit initial distributions of the type $\delta(x-x_0)$.

It remains to give the explicit solution for the expansion function $\Omega_2(x)$ of equation (7.16). This is

$$\Omega_2(x) = \frac{\alpha(x)g(x)}{\alpha^2(x)+\pi^2} + \frac{\mathrm{e}^{\Gamma(x)}}{[\alpha^2(x)+\pi^2]^{1/2}}\mathrm{Pv}\int_1^\infty \frac{\mathrm{e}^{-\Gamma(y)}g(y)z'(y)\,\mathrm{d}y}{[\alpha^2(y)+\pi^2]^{1/2}[z(y)-z(x)]}. \qquad (7.24)$$

Here the functions α, g and θ take the same forms as earlier, while Γ is re-interpreted as

$$\Gamma(x) = \frac{1}{\pi}\mathrm{Pv}\int_0^\infty \frac{\theta(y)z'(y)\,\mathrm{d}y}{z(y)-z(x)}. \qquad (7.25)$$

† Although in the references cited the integral operators are described for other domains such as $(-1, +1)$, translation of the results for the infinite interval $(1, \infty)$ presents no difficulty. We may note that, since $\Omega_2(\lambda)$ vanishes in the interval $(0, 1)$ the lower limit in equation (7.20) can equally well be written as zero.

8. Fundamental solution of the initial-value problem

As usual in linear relaxation studies, we focus attention on the 'fundamental' initial condition

$$P(x, 0) = \delta(x-x_0), \tag{8.1}$$

noting that virtually all interesting cases may be treated by superposition of results for this choice.

The separation into odd and even components now reads

$$P_{\text{ev}}(x, 0) = \tfrac{1}{2}[\delta(x-x_0)+\delta(x+x_0)] \tag{8.2}$$

$$P_{\text{od}}(x, 0) = \tfrac{1}{2}[\delta(x-x_0)-\delta(x+x_0)] \tag{8.3}$$

and we seek to construct solutions of type (7.4) and (7.5) through the two expansion functions $\omega_1(\lambda)$ and $\omega_2(\lambda)$. The even component is again determined more straightforwardly and we concentrate on this first.

On inserting (8.2) into the right-hand side of (7.9) it is found that the crucial term in the result is the indefinite integral

$$\sigma(x, x_0) = \int^x (\operatorname{sgn} y)[\delta(y-x_0)+\delta(y+x_0)]\, \mathrm{d}y.$$

This can be interpreted by symbolic integration by parts to give

$$\begin{aligned}\sigma(x, x_0) &= \tfrac{1}{2}(\operatorname{sgn} x)[\operatorname{sgn}(x-x_0)+\operatorname{sgn}(x+x_0)] \\ &= \begin{cases} 0; & |x| < |x_0| \\ 1; & |x| > |x_0| \end{cases}\end{aligned} \tag{8.4}$$

and it follows that

$$\int^{\infty} (\operatorname{sgn} x) P_{\text{ev}}(x, 0)\, \mathrm{d}x = \tfrac{1}{2}. \tag{8.5}$$

The even expansion function then becomes

$$\omega_1(x) = \frac{\delta(x-x_0)+\delta(x+x_0)}{[z'(x)]^2} - \frac{\mathrm{e}^{-x^2}\sigma(x, x_0)}{[z'(|x|)]^3}. \tag{8.6}$$

Substituting this into (7.6), we arrive at the relatively simple result

$$\begin{aligned}P_{\text{ev}}(x, \tau) &= \pi^{-1/2}\, \mathrm{e}^{-x^2} + \tfrac{1}{2}\{\delta(x-x_0)+\delta(x+x_0)\}\, \mathrm{e}^{-z(x_0)\tau} \\ &\quad - \begin{cases} \mathrm{e}^{-x^2} U(x_0, \tau); & |x| \leqslant |x_0| \\ \mathrm{e}^{-x^2} U(x, \tau); & |x| > |x_0| \end{cases}\end{aligned} \tag{8.7}$$

in which the function $U(x, \tau)$ has been defined

$$U(x, \tau) = \frac{\mathrm{e}^{-z(x)\tau}}{|z'(x)|} - 2\int_{|x|}^{\infty} \frac{\exp[-y^2 - z(y)\tau]}{[z'(y)]^2}\mathrm{d}y. \tag{8.8}$$

Although, as written, $U(x, \tau)$ appears to be singular at $x = 0$, the singularities in the two terms in fact cancel and we find, on separating the case $\tau = 0$, that it takes the simpler form

$$U(x,\tau) = \begin{cases} \pi^{-1/2}; & \tau = 0 \\ \tau \int_{|x|}^{\infty} e^{-z(y)\tau}\, dy; & \tau > 0. \end{cases} \tag{8.9}$$

It is easily verified that

$$\int_{-\infty}^{+\infty} P_{ev}(x,\tau)\, dx = 1$$

for all $(0 \leqslant \tau \leqslant \infty)$, while the correct limiting behaviour $P(x, 0) = \delta(x-x_0)$ and $P(x, \infty) = \pi^{-1/2} \exp(-x^2)$ is evident.

As anticipated, the odd solutions present a much more difficult problem. We can only note that the odd component is given by

$$\begin{aligned} P_{od}(x,\tau) = & -\tfrac{1}{2}[z'(x)]^2 (\operatorname{sgn} x) R(\infty, x)\, e^{-z(x)\tau}\Omega_2(x) \\ & - e^{-x^2}(\operatorname{sgn} x) \int_0^{|x|} \Omega_2(y) R(\infty, y) z'(y)\, e^{-z(y)\tau}\, dy \\ & + e^{-x^2} \int_0^{\infty} \Omega_2(y) R(x, y) z'(y)\, e^{-z(y)\tau}\, dy \end{aligned} \tag{8.10}$$

with the function $\Omega_2(x)$ to be determined through equation (7.21). Introducing the odd component of the delta function, we then find that the function $g(x)$ appearing there takes the form

$$g(x) = \tfrac{1}{2}\{\operatorname{sgn}(x-x_0) - \operatorname{sgn}(x+x_0)\} - \tfrac{1}{2} e^{x^2} z'(x)\{\delta(x-x_0) - \delta(x+x_0)\}. \tag{8.11}$$

Beyond this there seems to be little possibility of obtaining a compact form for the evolution of $P_{od}(x, \tau)$ similar to equation (8.7). It may, however, be verified that the solution contains a transient singular term of the form

$$[\delta(x-x_0) - \delta(x+x_0)]\, e^{-z(x_0)\tau}$$

plus others which vanish correctly for $\tau \to 0$ and $\tau \to \infty$.

9. The speed relaxation

It seems time to return to the physics of the problem. Clearly a main feature of the results is the contrast between the relative simplicity of the *even* initial-value solutions and the considerably more involved form of their *odd* counterparts. This evidently has its origin in the difference between the straightforward relaxation of *speed*, or kinetic energy, by 'instant thermalization' and the much more complex equilibration of *direction* in the ensemble of test particles. This latter process will be characterized by a tendency to *anti*correlation of direction before and after collisions, moving particles being appreciably more likely to make head-on collisions (type A in figure 1) rather than knocking-on collisions (types B and C). At the same time the relaxation in the speed variable proves more subtle than the picture of 'instant thermalization' would suggest; because both the waiting time between collisions and the probable velocity of the next collision partner are sensitive functions of the test particle's velocity, the latter having the modified maxwellian form reflected in the kernel (5.6).

Nevertheless, the main visible content of the model is to be found in the *even* solutions and the speed, or energy, relaxation which they express. We shall concentrate on this aspect for the remainder of the paper. Writing the speed distribution function with the help of (5.7) and the results of the previous section we find that

$$P(|x|, \tau) = 2\pi^{-1/2}\,\mathrm{e}^{-x^2} + \delta(|x|-|x_0|)\,\mathrm{e}^{-z(x_0)\tau} - \begin{cases} 2\,\mathrm{e}^{-x^2}U(|x_0|, \tau); & |x| \leqslant |x_0| \\ 2\,\mathrm{e}^{-x^2}U(|x|, \tau); & |x| > |x_0| \end{cases} \tag{9.1}$$

with the function $U(x, \tau)$ defined as before and the initial condition modified to $P(|x|, 0) = \delta(|x|-|x_0|)$. (Note that the normalization is now over the range $0 < |x| < \infty$.)

The physical interpretation of the various terms is quite clear. The first is the equilibrium maxwellian and the second represents correctly the decay of the initial delta function. This component alone decays by a simple Poisson process with time constant $z(x_0)^{-1}$—evidently the mean waiting time for particles to suffer their first collision. Finally the terms with the function U give the more involved transient reflecting the spread of velocities after the first collision. Again the solution conserves probability at all times and reduces to the singular initial condition as time tends to zero.

The character of the terms in the function U may be made clearer on observing the form the solution takes for the special case $1 \leqslant x_0 \ll x < \infty$. Under these conditions, the asymptotic expansion for erf(x) may be used to give $z(x) \underset{x\to\infty}{\sim} \pi^{1/2}x$. The solution then takes on the simpler form

$$P(|x|, \tau) = \exp(-\pi^{1/2}|x_0|\tau)\delta(|x|-|x_0|) + \begin{cases} 2\pi^{1/2}\,\mathrm{e}^{-x^2}[1-\exp(-\pi^{1/2}|x_0|\tau)]; & |x| \leqslant |x_0| \\ 2\pi^{1/2}\,\mathrm{e}^{-x^2}[1-\exp(-\pi^{1/2}|x|\tau)]; & |x| > |x_0|. \end{cases} \tag{9.2}$$

Surprisingly perhaps, this approximation still conserves probability for all times and gives the correct limiting behaviour for both $\tau = 0$ and $\tau \to \infty$. Further inspection shows that it should also be a satisfactory approximation in the short time regime $\tau \ll 1$, whatever the relative values of x and x_0—for this reason the expression for $|x| \leqslant |x_0|$ is included above.

A selection of time dependent distribution functions computed from equation (9.1) is illustrated in figure 3. The curves show clearly that, with unit mass ratio, the Rayleigh relaxation process is effectively dominated by the distribution of waiting times for collision, no persistence of velocity being possible under these conditions in one dimension. In each case the delta function decays without tendency to spread in its neighbourhood, and it can be seen that, in general, the high-speed tail of the maxwellian is filled most rapidly, with equilibration following slowest at near-zero speeds.

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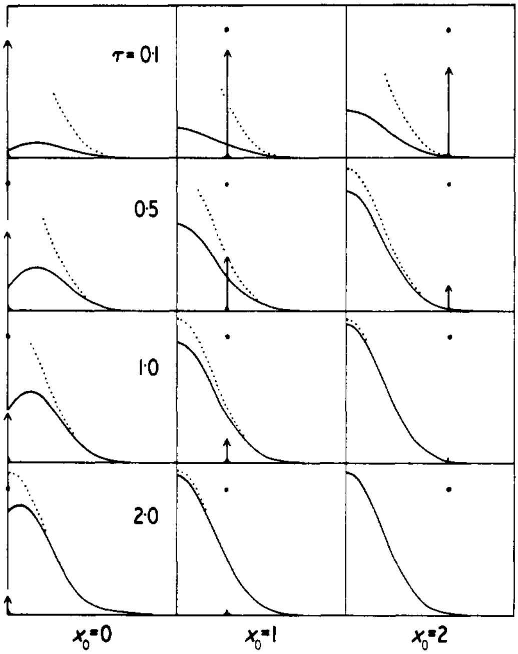

Figure 3. Relaxation of Rayleigh piston ensembles with initial δ distributions $P(x, 0) = \delta(x - x_0)$. The equilibrium maxwellian is shown dotted and the contribution of the delta function component is scaled to unity by the single dot. Note the increase in overall rapidity of thermalization with higher x_0 and the preferential filling of the high-speed tail of the gaussian at shorter times (equation (10.1)).

Appendix

A.1. The pseudofunction Pf. $R(x, \lambda)$

We shall explain, so far as possible without the apparatus of distribution theory, how the pseudofunction Pf. $R(x, \lambda)$ is to be interpreted and how the Hadamard finite part may be extracted when it acts on a given test function $\varphi(x)$.

Technically, the pseudofunction Pf. $R(x, \lambda)$ satisfying equation (2.10) is the *primitive*, or indefinite integral of the simpler generalized function Pf. $[z(x)-\lambda]^{-2}$, and its action on a test function $\varphi(x)$ is to be understood as

$$\langle \text{Pf. } R(x, \lambda), \varphi(x)\rangle = \text{Fp} \int_a^b R(x, \lambda)\varphi(x)\,\mathrm{d}x \qquad (a < x_\lambda < b) \tag{A.1}$$

where the prefix Fp indicates that the Hadamard finite part of the integral is to be taken. However, by the definition of the derivative of a distribution, the action of $R(x, \lambda)$ is more conveniently expressed as

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

where, as always, the test functions are assumed correctly behaved at the boundaries.

Inasmuch as equation (A.2) is the *definition* of the solution $R(x, \lambda)$ of the eigenvalue equations (2.10) and (3.3), we may use partial integrations to simplify integrals of type (A.2) without hesitation. The extraction of the finite part of the integral above is then carried out as follows. We write

$$\langle \mathrm{Pf.}\,[z(x)-\lambda]^{-2}, \varphi(x)\rangle = \lim_{\epsilon\to 0}\left[\left(\int_{z(a)}^{\lambda-\epsilon} + \int_{\lambda+\epsilon}^{z(b)}\right)\frac{F(z)\,\mathrm{d}z}{[z-\lambda]^2} - I(\epsilon)\right] \tag{A.3}$$

having put

$$F(z) = \varphi[y(z)]/(\mathrm{d}z/\mathrm{d}y) = \varphi[y(z)]/\pi^{1/2}\,\mathrm{erf}(y(z))$$

with $y(z)$ the inverse collision number function. $I(\epsilon)$ is the divergent part of the integral to be eliminated. We note that $F(z)$ is regular across the singularity, taking the value $F(\lambda) = \varphi(x_\lambda)/\pi^{1/2}\,\mathrm{erf}(x_\lambda)$, but is singular in the limit $\lambda \to 1^+$, $x_\lambda \to 0^+$.

Following Hadamard (see especially Zemanian 1965, §§ 1.4 and 2.5) $F(z)$ is expanded as

$$F(z) = F(\lambda) + F'(\lambda)(z-\lambda) + \psi(z)(z-\lambda)^2 \qquad (\lambda > 1) \tag{A.4}$$

where the function $\psi(z)$, regular at $z = \lambda$, can be expressed through the Taylor's theorem remainder formula.

On substituting the expression (A.4) into the integral, the logarithmic terms multiplying $F'(\lambda)$ are found to cancel and the remaining divergent term proves to be $I(\epsilon) = 2F(x_\lambda)/\epsilon$. Reverting to the integration over y, the required finite part can be written

$$\begin{aligned}\langle \mathrm{Pf.}\,[z(x)-\lambda]^{-2}, \varphi(x)\rangle &= \lim_{\epsilon\to 0}\left\{\left(\int_a^{x_\lambda-\epsilon} + \int_{x_\lambda+\epsilon}^{b}\right)\left[\frac{\varphi(y)\,\mathrm{d}y}{[z(y)-\lambda]^2} - \frac{2\varphi(x_\lambda)}{\epsilon[z'(x_\lambda)]^2}\right]\right\}\\ &= \int_a^b \left(\frac{\varphi(y)}{[z(y)-\lambda]^2} - \frac{\varphi(x_\lambda)}{[z'(x_\lambda)]^2(y-x_\lambda)^2}\right)\mathrm{d}y - \frac{\varphi(x_\lambda)}{[z'(x_\lambda)]^2}\left[\frac{b-a}{(b-x_\lambda)(x_\lambda-a)}\right].\end{aligned} \tag{A.5}$$

Now, although the solution of the singular equation (3.3) need never be considered in isolation, it is possible to arrive at a similar type of expression for Pf. $R(x, \lambda)$ itself. Thus, repeating the above analysis for the special case equivalent to putting $\varphi(y) = H(y)$ $H(x-y)$ (H the unit step function), we can identify $R(x, \lambda)$ itself with a function taking the values

$$\begin{aligned}R(x,\lambda) &\equiv \mathrm{Fp}\int_0^x \frac{\mathrm{d}y}{[z(y)-\lambda]^2}\\ &= \int_0^x \left(\frac{1}{(z(y)-\lambda)^2} - \frac{1}{[z'(x_\lambda)]^2(y-x_\lambda)^2}\right)\mathrm{d}y - \frac{1}{z'(x_\lambda)^2}\left[\frac{1}{x-x_\lambda} + \frac{1}{x_\lambda}\right].\end{aligned} \tag{A.6}$$

In this form, while $R(x, \lambda)$ remains uninterpreted for $x = x_\lambda$, the sense in which the differential equation (3.3) is satisfied for any $x \neq x_\lambda$ is fully apparent.

A.2. The integrals Q_1, Q_2, Q_3

Although the above results give insight into the nature of the singular eigenfunctions and the way they enter into the initial-value solution, they are not needed explicitly in the proofs of orthogonality and completeness. There are several points, however, where the subtler aspects of distribution theory cannot be overlooked. A crucial one is in the treatment of partial integrations involving a singularity. These occur particularly in the three integrals

$$Q_1(a, b, \lambda) = \mathrm{Fp}\int_a^b e^{-y^2}R(y, \lambda)\,dy$$

$$Q_2(a, b, \lambda) = \mathrm{Fp}\int_a^b y\,e^{-y^2}R(y, \lambda)\,dy$$

$$Q_3(a, b, \lambda, \lambda') = \mathrm{Fp}\int_a^b R(y, \lambda)R(y, \lambda')\,dy$$

where, in each case $a \leqslant x_\lambda \leqslant b$. When the singularity is outside the range of integration, naive partial integration using the facts that $e^{-y^2} = \frac{1}{2}z''(y)$, $ye^{-y^2} = -\frac{1}{4}z''(y)$ leads immediately to the results given (4.7), (4.8) and (6.6). The use of similar results for integration across the singularity requires proof that the extraction of finite parts does not leave additional terms in the final expressions. This supposes the validity of the generalized differentiation formula:

$$\frac{d}{dx}\mathrm{Pf.}\,H(x-a)H(b-x)[z(x)-\lambda]^{-1}$$
$$= -\mathrm{Pf.}\,H(x-a)H(b-x)z'(x)[z(x)-\lambda]^{-2} \qquad (\alpha \leqslant x_\lambda \leqslant b). \tag{A.7}$$

Standard results for the simpler functions Pf. x^{-1} and Pf. x^{-2} (Zemanian 1965, § 2.5, equations (23) and (24)) suggest that this relation should hold provided that the singularity is not at an end point of the range. A detailed analysis of the ϵ limit in the corresponding partial integration with a test function shows that the equivalence (A.7) is, in fact, correct for the open interval $a < x_\lambda < b$. If x_λ is at either end point, however, additional constant terms *do* arise in a manner given by the modified differentiation rule:

$$\frac{d}{dx}\mathrm{Pf.}\,H(x-x_\lambda)H(b-x)[z(x)-\lambda]^{-1}$$
$$= -\mathrm{Pf.}\,H(x-x_\lambda)H(b-x)z'(x)[z(x)-\lambda]^{-2}$$
$$+\frac{1}{z'(x_\lambda)}\delta'(x-x_\lambda)-\frac{z''(x_\lambda)}{2z'(x_\lambda)^2}\delta(x-x_\lambda) \tag{A.8}$$

and a similar result, but with change of sign of the singular terms when $x_\lambda = b$. Thus the two cases combined yield (A.7) with cancellation of the singularities. These results allow us to manipulate the Q integrals according to the rules of ordinary partial integration whenever x_λ is an interior point, while at the same time making quite explicit the delta singularities which appear in the integrals $Q_1(x)$ and $Q_2(x)$ as $x \to x_\lambda$. However, although end point singularities appear if the limit $\lambda \to \lambda'$ is imposed at any stage of the proof of orthogonality given in § 6, our particular arrangement of the intervals of integration enables us to carry all singularities except the crucial $\delta(\lambda-\lambda')$ implicitly in singular integrals which in the end result cancel.

References

Cercignani C 1969 *Mathematical Methods in Kinetic Theory* (New York: Plenum Press)
Guernsey R L 1960 *PhD Thesis* University of Michigan
Hoare M R 1971 *Adv. chem. Phys.* **20** 135–214
Hoare M R and Rahman M 1973 *J. Phys.* A: *Math., Nucl. Gen.* **6** 1461–78
Jepsen D W 1965 *J. math. Phys.* **6** 405–13
Jones D S 1966 *Generalized Functions* (London: McGraw-Hill)
Lebowitz J L, Percus J K and Sykes J 1968 *Phys. Rev.* **171** 224–35
Mushkhelishvili N I 1953 *Singular Integral Equations* (Gronigen: Nordhoff)
Schwartz L 1966 *Théorie des Distributions* (Paris: Hermann)
Tokizawa M 1970 *J. math. Phys.* **10** 1834–41
Tricomi F G 1957 *Integral Equations* (New York: Interscience)
Wu T-Y 1966 *Kinetic Equations of Gases and Plasmas* (Reading Mass.: Addison-Wesley)
Zemanian A H 1965 *Distribution Theory and Transform Analysis* (New York: McGraw-Hill)