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On the spectral theory of Rayleigh's piston
I. The discrete spectrum

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Abstract. The classic problem of Rayleigh's piston is reconsidered in the light of modern transport theory. We investigate the velocity relaxation of a one-dimensional ensemble of test particles immersed in a similar heat bath at arbitrary mass ratio γ, and obtain a new reduction of the integral collision operator to an infinite-order differential expansion more tractable than the conventional expression in powers of the mass ratio. In this way we prove that the number of nonzero discrete eigenvalues of the Rayleigh collision operator is always bounded for finite mass ratio, being in fact zero for the special case $\gamma = 1$. By truncation of the collision operator expansion, a tentative bound is then obtained which suggests (subject to an unproved positive-definiteness condition) that the emptiness of the discretum actually extends over at least the mass ratio region

$$\{3(\sqrt{2}-1)\}^{-1} < \gamma < 3(\sqrt{2}-1).$$

The limit $\gamma \to 0$ may be studied and gives a novel approach to Rayleigh's original solution under conditions of brownian motion.

1. Introduction

'Rayleigh's piston', arguably the simplest conceivable model in statistical dynamics, is remarkably little understood in spite of notable advances in transport theory which, 80 years after Baron Rayleigh's original formulation (Strutt 1891), seem to have overtaken this deceptively trivial-looking problem.

Translated into contemporary language and generalized somewhat, the Rayleigh model may be specified as follows. Consider an ensemble of test particles, mass M, constrained to move in one dimension and responding to random, impulsive collisions with a gas of heat-bath particles, mass m, having temperature T (figure 1). What is the evolution of a space and velocity distribution function $P(V, r, t)$ for the test particles from some given initial condition $P(V, r, 0)$? More simply—and as in the original version—what is the evolution of the velocity distribution $P(V, t)$ for the corresponding spatially-homogeneous system? To these questions we may add others of more modern interest. What is the velocity autocorrelation function $S_V(t)$ for equilibrium fluctuations in the ensemble, or equivalently its power spectrum $J_V(\omega)$? What is the space–time correlation function $G(r, t)$ for initial maxwellian velocities?

A discussion of some aspects of these problems will be found in the classic papers by Uhlenbeck and Ornstein (1930) and Wang and Uhlenbeck (1945) and in more recent reviews by Lax (1960) and Hoare (1971).

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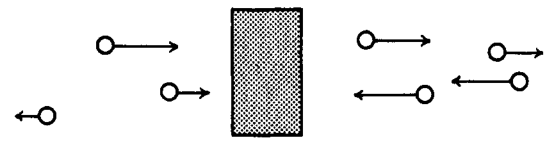

Figure 1. The Rayleigh piston. A piston of mass M and cross section σ undergoes random collisions with a one-dimensional heat bath of particles, mass m. The velocities of the heat-bath particles are Maxwell distributed at temperature T and their number density is n per unit volume.

Rayleigh's original treatment and its modern extensions (see eg Green 1951, Van Kampen 1961, Akama and Siegel 1965a, b) are concerned almost exclusively with the limiting case $M \gg m$, that is with very heavy test particles undergoing brownian motion in a light diluent gas. Only under these conditions is it possible to reduce the initial-value problem for $P(V, t)$ to that of a second-order integro-differential equation (the Rayleigh–Fokker–Planck equation) and obtain the well known closed form for the evolution of $P(V, t)$ to the equilibrium maxwellian:

$$P(V, \tau_R) = \left(\frac{M}{2\pi k_B T(1-e^{-2\tau_R})}\right)^{1/2} \exp\left(-\frac{M(V-V_0\,e^{-\tau_R})^2}{2k_B T(1-e^{-2\tau_R})}\right) \tag{1.1}$$

$$P(V, 0) = \delta(V - V_0)$$

$$\tau_R = 4n\sigma\left(\frac{2k_B T}{\pi M}\right)^{1/2} t.$$

Here σ is the cross-sectional area of the pistons and n the number density of the heat-bath particles.

Both the limitations of this solution and the lack of rigour in its derivation have been widely acknowledged. It is known to falsify the behaviour at short times whatever the mass ratio $\gamma = m/M$, while the supporting theory gives no indication of how small γ need actually be in order to give satisfactory solutions in the long-time regime. Even this minimal understanding must be sacrificed if the mass ratio is to be allowed arbitrary values in the range $0 < \gamma < \infty$, a possibility excluded at the outset in all the classical treatments from the point of view of brownian motion.

This general problem, for pistons of all possible relative masses and ensembles at all stages of evolution, will be explored in our present work. Considering first the spatially-homogeneous case, we begin by exhibiting a number of salient features of the integral collision operator $\mathscr{A}$ specifying the Markov process for $P(V, t)$ on the continuous space of velocity states $-\infty < V < \infty$. We go on to examine its spectral characteristics, restricting attention in this paper to the discrete part of the eigenvalue spectrum which, at least for certain ranges of γ, can be expected to dominate the solution after long times.

2. Preliminary formulation

The transport equation for the velocity distribution function $P(V, t)$ of an ensemble of Rayleigh pistons is of 'master equation' type and can be written

$$\frac{\partial}{\partial t}P(V, t) = \int_{-\infty}^{\infty} K(V', V)P(V', t)\,dV' - Z(V)P(V, t). \tag{2.1}$$

Here $K(V, V')$ is the transition kernel giving the probability flux from velocity V to dV' about V', while $Z(V)$ is the velocity-dependent collision number obtained by integration of K over all final states:

$$Z(V) = \int_{-\infty}^{+\infty} K(V, V')\, dV'. \tag{2.2}$$

Thus, if we wish to represent the initial-value problem in the compact form

$$\frac{\partial P}{\partial t} = \mathscr{A} P \tag{2.3}$$

the collision operator $\mathscr{A}$ must be taken as the symbolic integral operator

$$\mathscr{A} \equiv K(V', V) - Z(V)\delta(V - V').$$

The difficulty and subtlety of the Rayleigh piston problem derives from the second, singular term, whose presence rules out any possibility of a reduction of the solution to a standard exercise in the theory of Markov processes.

The explicit form of the transition kernel K was not given by Rayleigh, but has since been written by a number of workers (see eg Lebowitz and Bergmann 1957, Van Kampen 1961). A simple accounting of collisions with conservation of momentum and energy shows it to be

$$K(V, V') = \frac{n\sigma}{4}\left(\frac{m}{2\pi k_B T}\right)^{1/2}\left(\frac{1+\gamma}{\gamma}\right)^{2}|V - V'| \exp\left(-\frac{M}{8\gamma k_B T}\{V(\gamma - 1) + V'(\gamma + 1)\}^2\right). \tag{2.4}$$

Integration of this expression over all V' then leads to the following for the collision-number function $Z(V)$:

$$Z(V) = n\sigma\left[V \operatorname{erf}\left\{\left(\frac{m}{2k_B T}\right)^{1/2} V\right\} + \left(\frac{2k_B T}{\pi m}\right)^{1/2} \exp\left\{-\left(\frac{mV^2}{2k_B T}\right)\right\}\right]. \tag{2.5}$$

The equilibrium maxwellian for the ensemble is

$$f_M(V) = \left(\frac{M}{2\pi k_B T}\right)^{1/2} \exp\left(-\frac{MV^2}{2k_B T}\right), \tag{2.6}$$

from which we may see that the kernel $K(V, V')$ satisfies the detailed balance condition

$$f_M(V)K(V, V') = f_M(V')K(V', V). \tag{2.7}$$

It further follows from (2.2) and (2.7) that the maxwellian correctly satisfies the equilibrium condition $\mathscr{A} f_M = 0$.

Before analysing the transport equation further it is convenient to make the following transformations to reduced variables. Let

$$\tau = n\sigma\left(\frac{2k_B T}{\pi m}\right)^{1/2} t$$

$$x = \left(\frac{m}{2k_B T}\right)^{1/2} V$$

$$y = \left(\frac{m}{2k_B T}\right)^{1/2} V'.$$

$K(V, V')\,\mathrm{d}V'$ and $Z(V)$ reduce accordingly to

$$k(x, y)\,\mathrm{d}y = \left(\frac{1+\gamma}{2\gamma}\right)^2 |y-x| \exp\left(-\frac{1}{4\gamma^2}\{x(\gamma-1)+y(\gamma+1)\}^2\right) \mathrm{d}y \tag{2.8}$$

and

$$z(x) = \mathrm{e}^{-x^2} + \pi^{1/2} x \,\mathrm{erf}(x), \tag{2.9}$$

while the maxwellian becomes

$$f_\gamma(x) = (\pi\gamma)^{-1/2} \exp\left(-\frac{x^2}{\gamma}\right). \tag{2.10}$$

Finally we make a separation of the variables in the form

$$P(x, \tau) = (f_\gamma(x))^{1/2} \phi(x)\, \mathrm{e}^{-\lambda\tau} \tag{2.11}$$

and, on substituting back, obtain the following integral operator eigenvalue problem for $\phi(x)$ and λ:

$$(z(x) - \lambda)\phi(x) = \int_{-\infty}^{+\infty} g(x, y)\phi(y)\,\mathrm{d}y, \tag{2.12}$$

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

$$g(x, y) = \mu |y-x| \exp\{-\tfrac{1}{2}(x^2+y^2) - \rho(y-x)^2\} \tag{2.13}$$

with μ and ρ defined by

$$\mu = \tfrac{1}{4}(1+1/\gamma)^2; \qquad \rho = \tfrac{1}{4}(1/\gamma^2 - 1). \tag{2.14}$$

The kernel $g(x, y)$ proves to be square integrable on $(-\infty, \infty)$ and, in fact, gives the norm

$$\|g\|^2 = \iint_{-\infty}^{+\infty} (g(x, y))^2\,\mathrm{d}x\,\mathrm{d}y = \frac{\pi}{16}\gamma^3 \left(1+\frac{1}{\gamma}\right)^4. \tag{2.15}$$

A scale drawing showing the characteristic shape of the kernel $k(x, y)$ is given in figure 2.

The singular character of the initial-value problem now shows itself in equation (2.12) through the term $(z(x)-\lambda)$, which may evidently vanish at points x_λ satisfying the condition $z(x_\lambda) = \lambda$, for given λ. As a result, the composition of a general solution from terms of type (2.11) presents unusual difficulties. The most relevant of these will be outlined in the following section.

3. General properties of the transport equation

The general properties of integro-differential equations of the type (2.1) have only been elucidated in comparatively recent time, largely through the work of theorists in the fields of plasma physics and neutron transport theory. Nevertheless, thanks to Van Kampen (1955), Case (1959, 1960), Koppel (1963), Ferziger (1965), Kuščer and Corngold (1965, 1966) and others (for reviews see Hoare 1971 and Williams 1971) the broad characteristics of the resulting initial-value solutions are now quite well understood.

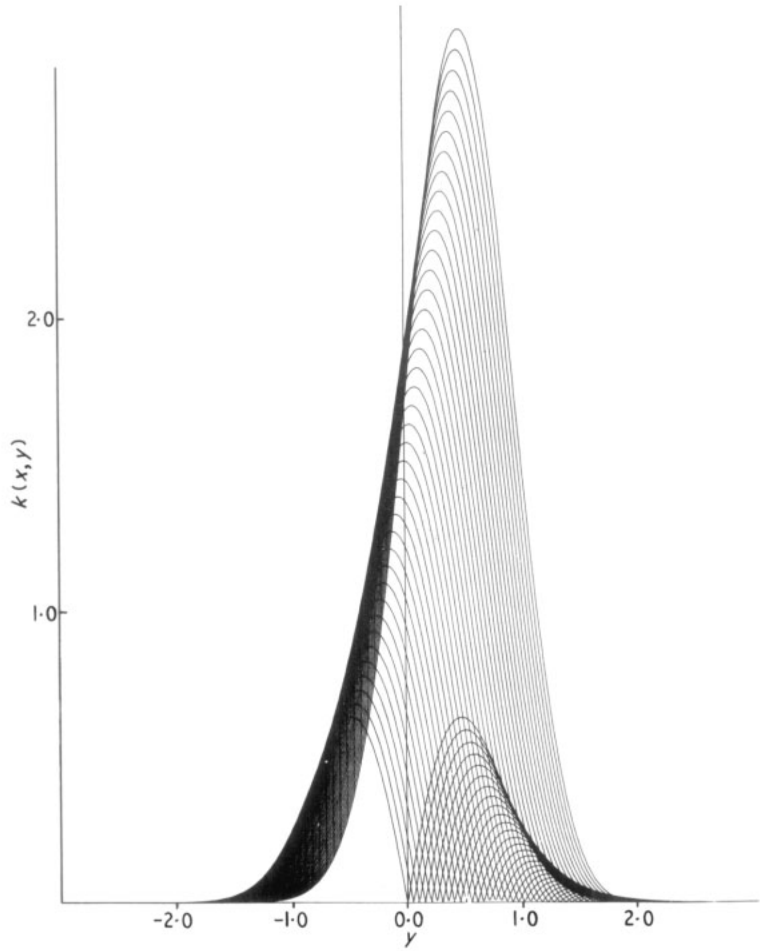

Figure 2. The Rayleigh kernel in reduced velocities (equation (2.8)). The family of curves shows the value of $k(x, y)$ as a function of y with x increasing from zero in increments of 0·05, for the particular mass ratio $\gamma = 0{\cdot}5$. The separate curves may be identified by their cusps on the horizontal axis at $x = y$. The curves for negative x are omitted since these are symmetrical about the vertical axis by virtue of $k(-x, y) = k(x, -y)$. As $\gamma \to 0$ the two peaks sharpen and encroach arbitrarily close at each side of the origin.

Briefly, it is now realized that the evolution of a distribution function $P(x, \tau)$ governed by a transport equation of the present type must be expressed in the following way:

$$P(x, \tau) = P(x, \infty) + \sum_k a_k \Phi_k(x)\, e^{-\lambda_k \tau} + \int_{\lambda \in C} a(\lambda)\Phi(x, \lambda)\, e^{-\lambda\tau}\, d\lambda. \tag{3.1}$$

The first term on the right is the equilibrium maxwellian $f_\gamma(x)$ and the transient terms which follow involve respectively the discrete spectrum λ_k and the continuous spectrum λ of the collision operator $\mathscr{A}$. The functions Φ are eigenfunctions, to be determined through solution of the singular integral equation $\mathscr{A}\Phi = \lambda\Phi$ and related to those of equation (2.12) by $\Phi = f_\gamma^{1/2}\phi$. The equilibrium eigenvalue $\lambda_0 = 0$ is always present, so long as particles are conserved, and accounts for the maxwellian term. The constants a_k and the function $a(\lambda)$ must be fitted according to the initial distribution $P(x, 0)$, a process only possible if the set of all eigenfunctions, for both discrete and continuous λ can be demonstrated to be *complete* for a sufficiently inclusive function space. The reality of all eigenvalues is guaranteed by the detailed balance condition which, in the appropriate form, can always be used to obtain a symmetric eigenvalue equation such as (2.12) above. Positive-definiteness of the spectrum, and hence boundedness of solutions, is likewise guaranteed by the detailed-balance condition plus the special relationship (2.2) between $k(x, y)$ and $z(x)$.

In general, the continuum C fills that part of the positive real line for which a root x_λ exists giving $z(x_\lambda)-\lambda = 0$. In the Rayleigh problem, with time scaled as above, this is evidently possible for all $\lambda \geqslant z(0) = 1$, so that the continuum fills the whole interval $(1, \infty)$. The discretum, $0 < \lambda < 1$ in the Rayleigh case, may, in general, either be empty, except for the single $\lambda_0 = 0$, or contain a finite number of eigenvalues, or an infinite number, necessarily with a point of accumulation.

The continuum eigenfunctions $\Phi(x, \lambda)$ are not square integrable and are normally singular distributions in the sense of Schwartz; so long as they are present, the discrete eigenfunctions, even though possibly infinite in number, do not form a complete set, and the solution of the form (3.1) without the integral term can never be fully accurate at any stage of the evolution. Nevertheless, the deficient solution may still tend to an arbitrarily good approximation in a particular time regime for which the 'continuum modes' $\exp(-\lambda\tau)$ become negligible. Thus, in cases such as the present one, in which the continuum is bounded from below, transients $\exp(-\lambda_k\tau)$ with $\lambda_k < 1$ will rapidly dominate in the 'aged' system with reduced time appreciably greater than unity—provided always that the discretum does not prove to be empty.

With these general considerations in mind, we shall describe the transformation of the singular eigenvalue problem (2.12) into an alternative form which provides valuable insight into the nature of the discrete spectrum and its functional dependence on the mass-ratio parameter γ. The first step will be to carry out a Fourier transformation in the velocity variable leading to the removal of the integral operator term and its replacement by a differential operator expression of infinite order. This version of the eigenvalue problem retains its singular character and implies no restriction on the allowed range of γ. In § 6 a second-order differential operator approximation to this is derived which, while retaining singular character, leads to definite numerical predictions of the discrete eigenvalues, which prove to be either zero or finite in number according to the region of γ. In § 7 these results are then used to prove the finiteness of the set λ_k for the unrestricted operator and to suggest tentative bounds to their number and values. We conclude with a brief discussion of the special cases $\gamma = 1$ and $\gamma \to 0$.

4. The collision-number function $z(x)$

In addition to the general properties just considered, a number of simplifying features peculiar to the Rayleigh problem depend crucially upon characteristics of the collision-number function $z(x)$. It will be convenient to specify these before beginning our main analysis of equation (2.12).

We note that:

(i) $z(x)$ is single valued and analytic for all x in the range $(-\infty, \infty)$.
(ii) It is symmetric in x. $z(-x) = z(x)$.
(iii) It is monotonic increasing in $|x|$ from its minimum at $z(0) = 1$.

(iv) For large $|x|$, $z(x) \sim |x|$.
(v) For small x, $z(x) = 1+x^2+O(x^4)$.
(vi) $z(x)$ is infinitely differentiable with, in particular,

$$z'(x) = \pi^{1/2}\,\mathrm{erf}(x) \tag{4.1}$$

$$z''(x) = 2\exp(-x^2) \tag{4.2}$$

and higher derivatives given by the Hermite functions:

$$D^n z(x) = (-1)^n 2\exp(-x^2)H_{n-2}(x) \qquad (n \geqslant 2). \tag{4.3}$$

(vii) $z(x)$ satisfies the differential equation

$$z''(x)+2xz'(x)-2z(x) = 0 \tag{4.4}$$

and is expressible as a special case of the confluent hypergeometric function

$$z(x) = {}_1F_1(-\tfrac{1}{2},\tfrac{1}{2};\,-x^2) \tag{4.5}$$

with

$${}_1F_1(a,b;x) = \sum_{k=0}^{\infty} \frac{(a)_k}{(b)_k}\frac{x^k}{k!} \tag{4.6}$$

($(a)_k = a(a+1)(a+2)\ldots(a+k-1)$).

(viii) The mean collision number per particle at equilibrium is given in the τ time scale by

$$z_{00} = \int_{-\infty}^{+\infty} z(x) f_\gamma(x)\,dx = (1+\gamma)^{1/2}. \tag{4.7}$$

A scale drawing of the function $z(|x|)$ is given in figure 3.

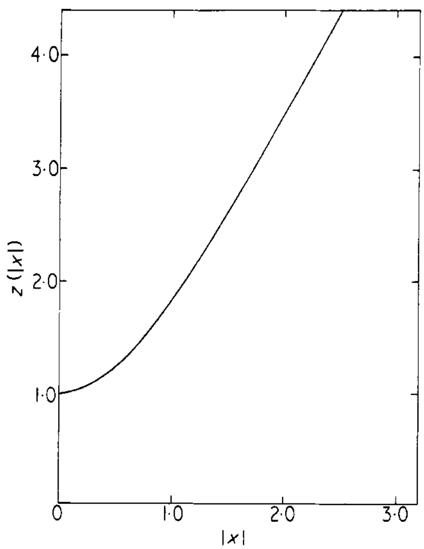

Figure 3. The collision-number function $z(|x|)$ for Rayleigh pistons in terms of reduced speeds (equation (2.9)). The velocity collision-number curve is the same with symmetric reflection about the y axis.

5. Reduction and Fourier transformation

It will prove convenient to treat the eigenvalue problem (2.8) first under the mass-ratio condition $\gamma < 1$ (the Rayleigh regime), afterwards modifying our discussion slightly to cover the range $\gamma > 1$ (the Lorentz regime). The special case $\gamma = 1$ may be considered separately.

A key step in the analysis of equation (2.12) is the recognition that, with slight modification of the eigenfunctions $\phi(x)$, the integral operator term on the right may be cast into the form of a convolution. Thus a Fourier transformation is indicated.

Writing

$$\psi(x) = \exp(-\tfrac{1}{2}x^2)\phi(x) \tag{5.1}$$

the eigenvalue condition reduces to

$$(z(x)-\lambda)\,e^{x^2}\psi(x) = \int_{-\infty}^{+\infty} B(y-x)\psi(y)\,dy = B(x) * \psi(x) \tag{5.2}$$

with $B(x)$ defined by

$$B(x) = \mu|x|\,e^{-\rho x^2}. \tag{5.3}$$

Before taking advantage of the convolution, however, we must assure ourselves, not only of the existence of the transform of $\psi(x)$, but also of that of the term $z(x)\,e^{x^2}\psi(x)$. This demands that we satisfy both the normal condition, that $\psi(x)$ be square integrable:

(i) $\qquad \psi(x) \in L_2(-\infty, \infty),$

and the considerably stronger one that

(ii) $\qquad z(x)\,e^{x^2}\psi(x) \in L_2(-\infty, \infty).$

Given (i) and the property that $z(x)$ is analytic and behaves as $|x|$ as $|x| \to \infty$, a sufficient condition for (ii) is that

(iii) $\qquad \psi(x) \underset{x\to\infty}{\sim} \exp\{-x^2(1+\epsilon)\}, \qquad (\epsilon > 0).$

Both conditions (i) and (iii) appear reasonable in as much as we are dealing with solutions having λ in the discretum $\lambda < 1$, while moreover the equilibrium solution $\psi_0(x)$ for $\lambda = 0$ undoubtedly satisfies both so long as $\gamma < 1$:

$$\psi_0(x) = \exp\left\{-x^2\left(\frac{1}{2}+\frac{1}{2\gamma}\right)\right\} = \exp\left\{-x^2\left(1+\frac{1-\gamma}{2\gamma}\right)\right\}. \tag{5.4}$$

Under these conditions we are then allowed to conclude that

(iv) $\qquad (1+|x|^n)\psi(x) \in L_2(-\infty, \infty)$

and hence that the Fourier transform is n times differentiable with all derivatives, as well as the original transform, tending to zero at infinity (see eg Titchmarsh 1937, p 174).

Let us denote the Fourier transform operation by $\mathscr{F}[\psi(x)] = \tilde{\psi}(k)$. Considering first the left-hand side of equation (5.2) we see that the transform may be obtained by writing this in the series form (4.5) and applying Kummer's relation (Erdelyi *et al* 1953, vol 1, p 253) to give

$$z(x)\,e^{x^2} = e^{x^2}{}_1F_1(-\tfrac{1}{2},\tfrac{1}{2};-x^2) = {}_1F_1(1,\tfrac{1}{2};x^2).$$

Thus, since $\mathscr{F}[x^{2m}\psi(x)] = (-1)^m D^{2m}\tilde{\psi}(k)$ ($D \equiv \mathrm{d}/\mathrm{d}k$), the two transforms may be written symbolically in terms of the gaussian and confluent hypergeometric operators. Thus

$$\mathscr{F}[\mathrm{e}^{x^2}\psi(x)] = \mathrm{e}^{-D^2}\tilde{\psi}(k) \tag{5.5}$$

and

$$\mathscr{F}[z(x)\,\mathrm{e}^{x^2}\psi(x)] = {}_1F_1(1, \tfrac{1}{2}; -D^2)\tilde{\psi}(k). \tag{5.6}$$

Turning now to the right-hand side of the equation, we see that the transformation of the integral may be achieved through the standard result:

$$\int_0^\infty t\exp(-at^2)\cos(kt)\,\mathrm{d}t = \frac{1}{2a}{}_1F_1(1, \tfrac{1}{2}; -k^2/4a) \tag{5.7}$$

(Erdelyi 1954, vol 1, p 15). Using this we obtain from the convolution

$$\mathscr{F}[B(x) * \psi(x)] = \left(\frac{1+\gamma}{1-\gamma}\right){}_1F_1(1, \tfrac{1}{2}; -k^2/4\rho)\tilde{\psi}(k). \tag{5.8}$$

This may also be reduced to a compact symbolic form by use of the confluent hypergeometric operator. Noting the Rodriguez formula

$$D^{2m}\exp(-b^2k^2) = b^{2m}\exp(-b^2k^2)H_{2m}(bk) \tag{5.9}$$

where $H_n(bk)$ is the Hermite polynomial of order n, and that there exists the expansion

$$(1+t)^{-a}{}_1F_1\left(a, \tfrac{1}{2}; \frac{x^2t}{1+t}\right) = \sum_{m=0}^{\infty}\frac{(a)_m}{(2m)!}t^m H_{2m}(x) \tag{5.10}$$

(Erdelyi 1953, vol 2, p 216).

We find that the transform of the right-hand side of (5.2) can be written as

$$\mathscr{F}[B(x) * \psi(x)] = \exp(b^2k^2)\tilde{\psi}(k)\,{}_1F_1(1, \tfrac{1}{2}; -D^2)\exp(-b^2k^2) \tag{5.11}$$

with

$$b^2 = \frac{1}{2}\left(\frac{\gamma}{1+\gamma}\right). \tag{5.12}$$

In this way we arrive at the remarkable infinite-order differential equation

$$\lambda\,\mathrm{e}^{-D^2}\tilde{\psi}(k) = {}_1F_1(1, \tfrac{1}{2}; -D^2)\tilde{\psi}(k) - \exp(b^2k^2)\tilde{\psi}(k)\,{}_1F_1(1, \tfrac{1}{2}; -D^2)\exp(-b^2k^2). \tag{5.13}$$

This version of the eigenvalue problem, formal as it is, remains exact and preserves the singular character of the original integral equation. One essential property is, moreover, quite transparent—the equilibrium solution, derived from (5.1) as

$$\tilde{\psi}_0(k) = \mathscr{F}[\psi_0(x)] = \exp(-b^2k^2) \tag{5.14}$$

can be seen at a glance to satisfy it for $\lambda = 0$.

A number of possibilities suggest themselves for reducing this equation to a definite algorithm for obtaining numerical eigenvalues and eigenfunctions. One is to expand the latter as series in the Hermite functions $\exp(-b^2k^2)H_n(bk)$ and use known relationships for the effect of D^n and $\exp(-D^2)$ on these. The orthogonality property then leads, by integration, to an infinite-matrix eigenvalue problem for the expansion coefficients. The advantage of this method, as against a direct Rayleigh–Ritz expansion applied to the integral equation, seems, however, slight.

The main importance of equation (5.13) for our present investigation is that it opens the way to a systematic approximation procedure which provides the tool we are seeking for a qualitative analysis of the discrete spectrum. The first steps in this are described in the next section.

6. The second-order differential approximation

Since the collision-number function $z(x)$ has a minimum at $x = 0$ and is monotonic as $|x|$ increases, one would expect on the previous analysis that the eigenfunctions are perfectly well behaved except in the neighbourhood of the origin, where a sharp peak may develop. Physically this means that the interactions of the relatively slow-moving test particles with the heat bath are the dominant influence in the solution, particularly at times longer than the 'continuum relaxation time' $\tau^* = 1/z(0) = 1$. Thus, following previous studies of the spectra of more complicated three-dimensional kernels (see particularly Kuščer and Corngold 1966 and Kuščer and Williams 1967) it appears reasonable to concentrate attention on the behaviour of the eigenfunctions $\psi(x)$ in the neighbourhood of $x = 0$. Our first move is to show that the lowest-order 'low-velocity' approximation corresponds precisely to the procedure of truncating the operator expression (5.13) at terms in D^2.

Writing the left-hand side expression to lowest order with

$$z(x)\,e^{x^2} \simeq 1+2x^2; \qquad e^{x^2} \simeq 1+x^2 \tag{6.1}$$

and observing that these imply the corresponding Fourier transforms

$$\mathscr{F}[z(x)\,e^{x^2}\psi(x)] \simeq (1-2D^2)\tilde{\psi}(k) \tag{6.2}$$

and

$$\mathscr{F}[e^{x^2}\psi(x)] \simeq (1-D^2)\tilde{\psi}(k) \tag{6.3}$$

we see that the result of applying such an approximation is indeed equivalent to truncation of the operators ${}_1F_1(1, \frac{1}{2}; -D^2)$ and e^{-D^2} at the second derivative terms:

$${}_1F_1(1, \tfrac{1}{2}; -D^2) \simeq 1-2D^2; \qquad e^{-D^2} \simeq 1-D^2. \tag{6.4}$$

Applying these approximations consistently to the operators in equation (5.13), we obtain the relatively simple second-order differential equation†

$$\frac{d^2\psi}{dk^2}+\left(\frac{\lambda+4b^2}{2-\lambda}-\frac{8b^4k^2}{2-\lambda}\right)\psi = 0. \tag{6.5}$$

Making the substitutions

$$k = \nu\xi; \qquad \nu = \frac{(2-\lambda)^{1/4}}{2b}; \qquad c = \frac{\lambda+4b^2}{2b^2\{2(2-\lambda)\}^{1/2}} \tag{6.6}$$

† It should be noted here that the low-velocity approximation we have used here is somewhat different in character from that used by Kuščer and Corngold (1966) when treating the three-dimensional Wigner–Wilkins kernel for the hard-sphere gas. Their modification of the kernel is equivalent to restricting attention to transitions in a region where *both* x and $y \simeq 0$. By contrast, we assume that only x is small while y in effect retains its whole range $-\infty$ to ∞. The Kuščer–Corngold method does not, in fact, appear to work when applied to the Rayleigh kernel.

this then comes into the form of the Hermite equation

$$\frac{d^2\tilde{\psi}}{d\xi^2}+(c-\xi^2)\tilde{\psi} = 0. \tag{6.7}$$

For the solution to be Fourier invertible (meaning in the present context invertible into an $L_2(-\infty, \infty)$ function) it must be bounded at infinity, a condition which, as is well known, is only possible so long as

$$c = 2n+1; \qquad n = 0, 1, 2, \ldots. \tag{6.8}$$

The eigenfunctions are then

$$\tilde{\psi}_n(k) = \exp\left(-\frac{k^2}{2v_n^2}\right) H_n\left(\frac{k}{v_n}\right) \tag{6.9}$$

and give the Fourier inverse

$$\psi_n(x) = \exp(-\tfrac{1}{2}x^2 v_n^2)H_n(v_n x). \tag{6.10}$$

Here we refer to specific discrete eigenvalues v_n connecting with the original ones λ_n through $v_n = (2-\lambda_n)^{1/4}/2b$. The λ_n themselves, which are clearly approximations to the discrete spectrum of the integral operator in (2.12), are now determined through the conditions (6.6) and (6.8) as

$$\lambda_n = 4b^2[(2n+1)\{1+2b^2+b^4(2n+1)^2\}^{1/2}-b^2(2n+1)^2-1]. \tag{6.11}$$

Finally we note that the original eigenfunctions $\phi_n(x)$ are given by

$$\phi_n(x) = \exp\{-\tfrac{1}{2}x^2(v_n^2-1)\}H_n(v_n x) \tag{6.12}$$

to within a normalization factor.

Once again it is important to stress that, in contrast to other approximations such as the Rayleigh–Fokker–Planck equation (see § 9), the eigenvalue equation (6.5) remains singular in character and retains definite information about the continuum threshold. Taking the transition to singular solutions as indicated by the failure of the Fourier inversion, we see from (6.5) and (6.6) that this occurs as soon as v becomes complex, that is, for $\lambda > 2$. Thus the truncation procedure, while preserving the continuum solutions, appears to move their threshold from $\lambda^* = 1$ to $\lambda^* = 2$, a relatively minor effect compared to the removal to infinity brought about by the RFP operator†.

Returning now to the eigenvalue expression (6.11) we see that the condition for discreteness $\lambda < 1$ implies a definite limit to the number of such eigenvalues. Working

† Although treatment of the continuum solutions has been excluded here, we may note in passing that, for $\lambda > 2$, a different change of variables is called for. Putting

$$k = v\xi; \qquad v = \frac{(\gamma-2)^{1/4}}{2b}; \qquad c = \frac{\lambda+4b^2}{2b^2\{2(\lambda-2)\}^{1/2}}$$

we are led this time to the equation

$$\frac{d^2\tilde{\psi}}{d\xi^2}+(\xi^2-c)\tilde{\psi} = 0.$$

It is well-known that the spectrum of this equation is continuous and that the solutions are non-square-integrable (see Titchmarsh 1962, p 107).

this out we obtain an apparent bound to the total number of discrete eigenvalues, N, as a function of mass ratio:

$$N(\gamma) \leqslant \frac{1}{2\sqrt{2}}\left(\frac{1}{\gamma}+3-\sqrt{2}\right) \qquad (\gamma < 1). \tag{6.13}$$

At the same time we may extract a condition for emptiness of the discretum ($N \geqslant 1$) as follows:

$$\gamma \geqslant \frac{1}{3(\sqrt{2}-1)} = 0\text{·}8047\ldots. \tag{6.14}$$

Although both these bounds remain tentative, in the sense that they depend on the nature and direction of the change in the spectrum brought about by truncation of the full operators in equation (5.13), they are suggestive of two quite definite qualitative properties. (*a*) That the discrete spectrum is finite and shows no point of accumulation. (*b*) That there exists a range of mass ratio for which the discrete spectrum is entirely empty between $\lambda_0 = 0$ and $\lambda^* = 1$. If proved unconditionally, these properties would set the Rayleigh piston model apart from its higher-dimensional analogue, the hard-sphere gas, for which neither proposition holds. (See Kuščer and Corngold 1965, Hoare 1971.)

In the next section we shall go on to prove our most important result, namely that the *finiteness* of the discrete spectrum holds good for the complete Rayleigh operator. It will not be possible to prove here that condition (*b*) holds rigorously, or to demonstrate that the bound (6.13) is definitely not weakened on going to the full operator. Nevertheless, we are able to show that, for the special case $\gamma = 1$, the discretum is definitely empty ($N(1) = 0$) while, for $\gamma \to 0$, N becomes arbitrarily large.

Before continuing, however, we must settle the question of the Lorentz regime ($\gamma > 1$) for which the above proofs do not apply in the form given. Fortunately a simple modification suffices. To retain a negative exponent in the kernel as written in equation (2.9), the constant ρ must be replaced by $\rho' = \frac{1}{4}(1-1/\gamma^2)$. This leads to a different factor from the integration (5.7) and a modified independent variable in the resulting function ${}_1F_1$. However, on interpreting the equivalent of equation (6.5) it is found that all previous results are recovered, with the single difference that, wherever it occurs, the mass ratio γ is replaced by $1/\gamma$.

It follows that the bound (6.13) can be rewritten

$$N(\gamma) \leqslant \frac{1}{2\sqrt{2}}\{\max(\gamma, \gamma^{-1})+3-\sqrt{2}\} \tag{6.15}$$

while the condition for emptiness of the discretum becomes

$$\{3(\sqrt{2}-1)\}^{-1} \leqslant \gamma \leqslant 3(\sqrt{2}-1). \tag{6.16}$$

Since the extension to the regime $\gamma > 1$ can always be made in the manner described, we shall leave this to be understood throughout the proofs which now follow.

The approximate eigenvalues λ_n are plotted as functions of γ for the extended range in figure 4.

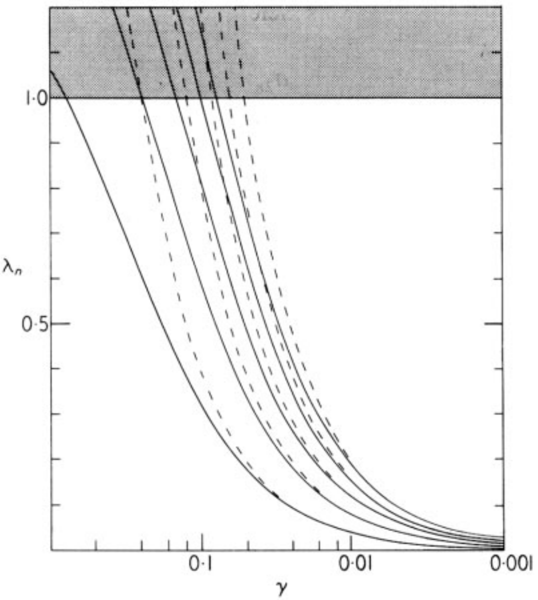

Figure 4. Approximate discrete eigenvalues for the Rayleigh piston according to equation (6.5) (full curves) and the Rayleigh–Fokker–Planck equation (broken curves). Only the first five nonzero eigenvalues are shown, for the mass-ratio range $\gamma < 1$. Note how the first eigenvalue enters the continuum top left, leaving the discretum empty in the range $0{\cdot}8047\ldots < \gamma < 1$. The full curves for $\gamma > 1$ are simply reflections about the vertical axis, on the logarithmic scale.

7. The full eigenvalue equation

In this section we shall carry out a qualitative analysis of the full differential eigenvalue equation and prove the main result that its discrete spectrum is finite.

We first split the operators $\exp(-D^2)$ and ${}_1F_1(1, \frac{1}{2}; -D^2)$ in the following manner:

$$e^{-D^2} = 1 - D^2 + \sum_{n=2}^{\infty} \frac{(-1)^n}{n!} D^{2n} \tag{7.1}$$

$${}_1F_1(1, \tfrac{1}{2}; -D^2) = 1 - 2D^2 + \sum_{n=2}^{\infty} \frac{(-1)^n}{(\frac{1}{2})_n} D^{2n}. \tag{7.2}$$

Repeating the substitutions (6.6) the operator equation (5.13) can now be written

$$c\psi(\xi) = T_0\psi + T_1\psi \tag{7.3}$$

where

$$T_0 = -\frac{d^2}{d\xi^2} + \xi^2 \tag{7.4}$$

and

$$T_1 = \frac{-v^2}{2-\lambda} \sum_{n=2}^{\infty} \frac{(-1)^n}{(\frac{1}{2})_n} b^{2n} H_{2n}(bv\xi) + \frac{v^2}{2-\lambda} \sum_{n=2}^{\infty} (-1)^n \frac{a_{2n}}{v^{2n}} \frac{d^{2n}}{d\xi^{2n}}. \tag{7.5}$$

Here the coefficients a_{2n} are given by

$$a_{2n} = \frac{1}{(\frac{1}{2})_n} - \frac{\lambda}{n!} \tag{7.6}$$

and the other parameters are as defined previously (for $\gamma < 1$). It is a simple matter to show that, for $\lambda < 1$, $a_{2n} > 0$ for all $n \geqslant 0$ and also that $a_{2n+2}/a_{2n} < 1$ for $0 < \lambda < 1$ and $n \geqslant 1$.

Let us now define a subspace S of $L_2(-\infty, \infty)$ consisting of functions $\psi(\xi)$ which satisfy the conditions

(i) $\psi(\xi)$ is infinitely differentiable.

(ii) $|\psi^{(q)}(\xi)| < C_q \exp(-m^2\xi^2)$

where $m^2 > \frac{1}{2}b^2v^2$ and C_q is a finite constant for all q. Here the superscript on ψ implies its qth derivative.

Now it can easily be seen that the truncated T_1 operator with N terms is self-adjoint, in as much as it is a series in the self-adjoint operator $-D^2$ and $T_1\psi$ is meaningful. These properties remain in the limit $N \to \infty$, $T_1\psi$ being still meaningful and the domain of T_1 again S by virtue of the conditions (i) and (iii).

The key result which we now have to prove is that T_1 is *bounded* in S. We have, for any $\phi(\xi) \in S$:

$$\begin{aligned}(\phi, T_1\phi) &= \int_{-\infty}^{+\infty} \mathrm{d}\xi\, \phi(\xi) T_1 \phi(\xi) \\ &= \frac{v^2}{2-\lambda} \sum_{n=2}^{\infty} \frac{(-1)^n}{(\frac{1}{2})_n} b^{2n} \int_{-\infty}^{+\infty} \mathrm{d}\xi\, H_{2n}(bv\xi)(\phi(\xi))^2 \\ &\quad - \frac{v^2}{2-\lambda} \sum_{n=2}^{\infty} (-1)^n \frac{a_n}{v^{2n}} \int_{-\infty}^{+\infty} \mathrm{d}\xi\, \phi(\xi) \frac{\mathrm{d}^{2n}\phi(\xi)}{\mathrm{d}\xi^{2n}}\end{aligned} \tag{7.7}$$

where we have made the assumption, justifiable in view of uniform convergence, that the integration and summation operations are interchangeable. Now

$$\int_{-\infty}^{+\infty} \mathrm{d}\xi\, \phi(\xi) \frac{\mathrm{d}^{2n}\phi(\xi)}{\mathrm{d}\xi^{2n}} = (-1)^n \int_{-\infty}^{+\infty} \mathrm{d}\xi (\phi^{(n)}(\xi))^2$$

and hence

$$\begin{aligned}&\sum_{n=2}^{\infty} (-1)^n \frac{a_n}{v^{2n}} \int_{-\infty}^{+\infty} \mathrm{d}\xi\, \phi(\xi) \left(\frac{\mathrm{d}^{2n}\phi(\xi)}{\mathrm{d}\xi^{2n}} \right) \\ &\qquad < \sum_{n=2}^{\infty} \frac{a_{2n}}{v^{2n}} C_n^2 \int_{-\infty}^{+\infty} \mathrm{d}\xi \exp(-2m\xi^2) < C^2 \sum_{n=2}^{\infty} \frac{a_{2n}}{v^{2n}} < \infty\end{aligned}$$

with C a finite constant $C_q < C < \infty$. In a similar way

$$\begin{aligned}&\left| \sum_{n=2}^{\infty} \frac{(-1)^n}{(\frac{1}{2})_n} b^{2n} \int_{-\infty}^{+\infty} \mathrm{d}\xi\, H_{2n}(bv\xi)(\phi(\xi))^2 \right| \\ &\qquad < C_0^2 \sum_{n=2}^{\infty} \frac{(-1)^n}{(\frac{1}{2})_n} b^{2n} \left| \int_{-\infty}^{+\infty} \mathrm{d}\xi H_{2n}(bv\xi) \exp(-2m^2\xi^2) \right| < \infty\end{aligned} \tag{7.8}$$

since $2m^2 > b^2v^2$ and $2b^2 < 1$. Hence $(\phi, T_1\phi)$ is finite and we can further write for the norm $\|T_1\| = t_1$ with t_1 a finite constant depending only on v. The limiting behaviour for large v is then easily seen to be

$$\|T_1\| = O(1/v^2). \tag{7.9}$$

We are now in a position to exploit the crucial theorem:

Let T_0 be self-adjoint and T_1 be symmetric. Then $T = T_0 + T_1$ is self-adjoint and moreover

$$\mathrm{dist}(\Sigma(T), \Sigma(T_0)) \leqslant \|T_1\|$$

where $\Sigma(T)$ and $\Sigma(T_0)$ are the spectra of T and T_0 respectively (Kato 1966, p 291)†.

But we have seen in the previous section that the spectrum of the truncated operator T_0 in (7.4) is finite in the discretum range $\lambda < 1$. The theorem just stated thus implies that the complete operator $T_0 + T_1$ has precisely the same behaviour.

The status of the other results derived in § 6, particularly the bounds (6.15) and (6.16), must now be considered. Obviously it would be desirable to show that, on addition of the perturbation T_1, the eigenvalues of the truncated operator T_0 are shifted upwards, in which case the bounds would stand and perhaps be improved. Unfortunately this would require us to show that T_1 is *positive definite*, a considerably more difficult proposition than the proof that it is bounded. We have not been able to discover such a proof and must therefore reluctantly leave the bounds as tentative ones so far as the spectrum of the full integral operator is concerned.

8. The special case $\gamma = 1$

Since we shall later study this special case in considerable detail in connection with the continuous spectrum, we shall only sketch here the proof of the important result that, when both test particle and heat-bath particles have equal mass, the discrete spectrum of the Rayleigh integral operator is empty.

The condition $\gamma = 1$ corresponds to the well known mechanical curiosity in which objects of symmetrical mass and shape simply exchange their respective velocities on colliding along their line of centres. At first sight this would appear to indicate that the test particles become thermalized according to a simple Poisson process with a single relaxation time. The equilibration of an ensemble with specified $P(V, 0)$ is, however, much more complicated than this, for the reason that the faster test particles tend to collide sooner and have an enhanced probability of making a head-on collision leading to a reversal of their direction. The resulting solution is far from trivial.

When we set $\gamma = 1$, the symmetrized kernel $g(x, y)$ takes the very simple form

$$g(x, y) = |x - y| \exp\{-\tfrac{1}{2}(x^2 + y^2)\}. \tag{8.1}$$

This has the character of a Green function for a second-order differential equation and the eigenvalue problem (2.12) is readily cast into this form on using the symbolic operations: $(\mathrm{d}/\mathrm{d}x)|x-y| = U(x-y)$ and $(\mathrm{d}^2/\mathrm{d}x^2)|x-y| = 2\delta(x-y)$. The result, which is somewhat similar to the Wigner–Wilkins equation for the hard-sphere gas (see Williams

† The function dist(,) is to be interpreted as taking the value $\max_i |\lambda_i - \lambda_i'|$ where λ_i, λ_i' are corresponding eigenvalues in the spectra under comparison.

1966, p 75) is found to be

$$\frac{d^2}{dx^2}\{(z(x)-\lambda)\exp(\tfrac{1}{2}x^2)\phi(x)\}-2\exp(-\tfrac{1}{2}x^2)\phi(x) = 0. \tag{8.2}$$

Using the result (4.2), one solution of this follows immediately as $\phi(x) = \exp(-\frac{1}{2}x^2)$, evidently corresponding to $\lambda = 0$. A second, independent solution can then be found, leading to the general solution

$$\phi(x, \lambda) = \exp(-\tfrac{1}{2}x^2)\left(A+B\int^x \frac{dy}{(z(y)-\lambda)^2}\right). \tag{8.3}$$

This is clearly singular for $\lambda > z(0) = 1$. Leaving aside the singular solutions, we concentrate here on the question of whether solutions of the integral eigenvalue equation with $\lambda < 1$, other than the trivial $\lambda_0 = 0$, can exist.

To decide this the solution (8.3) is substituted back into the integral equation and the conditions imposed on the two constants A and B are examined. After some manipulations, an identity is obtained which can only be satisfied by simultaneously fixing $A = B = 0$. Thus we are forced to conclude that the discretum is empty for $0 < \lambda < 1$ and that all transients in the relaxation problem arise from continuum modes with $\lambda \geqslant 1$. This is consistent with the tentative bound (6.16).

9. The Rayleigh–Fokker–Planck equation

Rayleigh's original solution (1.1) was obtained by an ingenious manipulation of the transport equation (2.1) using the condition $\gamma \ll 1$ to reduce its right-hand side to a second-order differential expression. His approximate equation, when rewritten in terms of our variables x and τ, takes the very simple form

$$\frac{1}{4\gamma}\frac{\partial P(x,\tau)}{\partial\tau} = \frac{\partial}{\partial x}(xP)+\frac{\gamma}{2}\frac{\partial^2 P}{\partial x^2}. \tag{9.1}$$

This clearly invites a further transformation of time scale by a factor involving the mass ratio: $\tau_R = 4\gamma\tau$ as in (1.1).

Subsequent workers have made Rayleigh's procedure more systematic, though scarcely more rigorous. In modern terms the above is seen as a special example of the Fokker–Plank equation, whose form may be prescribed in a well known way through the moments of the transition kernel $k(x, y)$ reduced to lowest order in γ. Nevertheless, despite considerable attention in the last thirty years (see particularly Kramers 1940, Moyal 1949, Keilson and Storer 1952, Van Kampen 1961, Akama and Siegel 1965a,b), very little can be said about the validity or accuracy of the symbolic replacement

$$(4\gamma)^{-1}\mathscr{A} \simeq \mathscr{R} = \frac{\gamma}{2}\frac{\partial^2}{\partial x^2}+x\frac{\partial}{\partial x}+1$$

in the full transport equation (2.1) with the Rayleigh kernel.

Although we hesitate to enter the general discussion of the foundations of the Fokker–Planck equation, it seems of interest to re-derive the Rayleigh solution, using the results of our § 7, and perhaps shed new light on the nature of the limiting processes involved.

Rayleigh's solution may be presented in eigenfunction form by noticing that the equation $\mathscr{R}\phi_n^{\mathrm{R}}(x) = \lambda_n^{\mathrm{R}}\phi_n^{\mathrm{R}}(x)$ has the complete set of solutions

$$\phi_n^{\mathrm{R}}(x) = \exp\left(-\frac{x^2}{\gamma}\right)H_n\left(\frac{x}{\gamma^{1/2}}\right) \tag{9.2}$$

with

$$\lambda_n^{\mathrm{R}} = 0, 1, 2 \ldots . \tag{9.3}$$

The initial-value solution for $P(x, 0) = \delta(x - x_0)$ then follows as

$$P(x, \tau_{\mathrm{R}}) = \exp\left(-\frac{x^2}{\gamma}\right)\sum_{n=0}^{\infty}(2^n n!)^{-1}H_n\left(\frac{x}{\gamma^{1/2}}\right)H_n\left(\frac{x_0}{\gamma^{1/2}}\right)\exp(-n\tau_{\mathrm{R}}). \tag{9.4}$$

The summation may be evaluated using Mehler's formula (Erdelyi 1953, vol 2, p 194) and yields the scaled form of equation (1.1) (cf Uhlenbeck and Ornstein 1930, p 839).

That this also follows from our development, can be seen on observing the effect of the limit $\gamma \to 0$ on the various quantities defined in § 7.

We observe first that

$$b^2 = \tfrac{1}{2}\gamma + \mathrm{O}(\gamma)$$

so that, interpreting equation (6.11) to lowest order,

$$\lambda_n = 4n\gamma + \mathrm{O}(\gamma^2),$$

in agreement with (9.3). (We note, however, the quite essential implication that n has a given, *finite* value throughout.) It then follows immediately that

$$\nu_n = \gamma^{-1/2}(1 + \mathrm{O}(\gamma)).$$

Entering these results into the solution (6.12) we evidently recover the Rayleigh eigenfunctions in the limit of small γ. What is more important, however, is that our previously-developed bound for the norm of the truncated part of the full Rayleigh operator can now be written

$$\|T_1\| = \mathrm{O}(\nu^{-2}) = \mathrm{O}(\gamma).$$

This result, though far short of a complete justification of the Rayleigh–Fokker–Planck equation, would seem to contain the essence of its validity as an approximation.

At the same time we can see why it has been possible for the authors of the treatments cited earlier to ignore the existence of the continuum altogether in their discussion of brownian motion. By scaling time in terms of the mass ratio, $\tau_{\mathrm{R}} = 4\gamma\tau$, the continuum transients $\exp(-\lambda\tau)$ with $\lambda > \lambda^* = 1$ are automatically suppressed in the limit $\gamma \to 0$. Needless to say this is a distortion of reality when γ is a small but finite quantity and the Rayleigh–Fokker–Planck equation is meant as a working approximation. In this case we are forced to recognize that, *in the Rayleigh time scale*, the continuum threshold is, in fact, only displaced to $\lambda^* = (4\gamma)^{-1}$ and that the eigenvalues λ_n^{R} must cross it and lose their normal significance for values of the index $n > (4\gamma)^{-1}$. This property, along with the systematic divergence between the eigenvalues from equation (9.1) and those of the alternative (6.5) is also illustrated in figure 4. Here it may be seen that, in general, the Rayleigh eigenvalues disappear into the continuum at lower values than do those of our equation, the discrepancy becoming increasingly marked for the smallest n values. In this respect, the general pattern of results from equation (6.5) is reminiscent of those obtained elsewhere in numerical Rayleigh–Ritz calculations on the three-dimensional hard-sphere system (see Hoare and Kaplinsky 1970).

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