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On the Spectrum of the Rayleigh Piston

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We make a rigorous study of the spectrum of the Rayleigh piston. Our main results are that one is dealing with a trace-class perturbation for all values of the mass ratio γ between test particles and heat bath particles and that apart from the ground state the discrete spectrum is empty for γ sufficiently near 1. We also show that the so-called Lorentz limit ($\gamma \to \infty$) is mathematically well defined and derive a qualitative statement on the discrete spectrum of the scattering operator for $\gamma \gg 1$.

KEY WORDS: Rayleigh piston; scattering operator; trace-class perturbation; discrete spectrum; Lorentz-limit.

I. INTRODUCTION

In recent years a considerable amount of effort has been spent on a classic of statistical mechanics—the Rayleigh piston (i.e., a one-dimensional array of test particles of mass M colliding at random with heat bath particles of mass m at temperature T)—in an attempt to come to grips with its full mathematical complexity (for a recent extensive bibliography of the problem and its ramifications see Ref. 1).

However, a great deal remains to be done even as regards qualitative properties of the model. With this paper we embark on a program of studying the qualitative and quantitative features which result from spectral analysis of the scattering operator canonically associated with each value of the mass ratio $\gamma = m/M$ between the two types of particles. Important first results have been obtained in Ref. 2. Since the model itself and the way of getting from the physics to the mathematical perturbation problem studied below have been described there and in numerous other texts (see, e.g., the review in Ref. 3), we shall not say anything about this here and shall from the start focus attention on the purely mathematical aspects of the problem.

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In Section 2 we shall define the problem, fix notation, and prove some technical results. In the following two sections we prove the main results of this paper: firstly, that in fact we are dealing with a trace-class perturbation for all values of γ; secondly we prove a conjecture put forward in Ref. 2, namely, that for a whole interval of values of γ containing the number 1 in its interior the only discrete eigenvector of the perturbed operator is the ground-state vector (which is unique). In the final section we then make a few remarks on the limits zero and infinity of γ and prove some basic results on the so-called Lorentz limit which does not seem to have attracted much attention so far in contrast to the Brownian limit.

The methods employed in this paper are quite straightforward and elementary; this, of course, does not mean that all pertinent questions can be answered in this fashion. The manipulation of improper integrals, taking of distributional derivatives, etc. will normally be done without explicit justification in order to keep the paper short; the interested reader can work things out for himself consulting standard textbooks if necessary. The background material on Hilbert space operators, sesquilinear forms, and their perturbations can all be found in Ref. 4, Chapters V, VI, and X. Let us finally mention that the three-dimensional analog of the Rayleigh piston (i.e., the neutron transport problem) has been studied in a similar way in Ref. 7.

2. PRELIMINARIES AND TECHNICALITIES

With γ defined as above define $\mu := (1+\gamma)(2\gamma)^{-1}$, i.e., $\gamma = (2\mu - 1)^{-1}$ and let

$$Z(x) := e^{-x^2} + 2x\,\mathrm{erf}(x) \qquad \text{with } \mathrm{erf}(x) = \int_0^x e^{-t^2}\,dt$$

Then Z is the corresponding (self-adjoint) multiplication operator on L^2 ($\mathbb{R}$). Next define $G : L^2 \to L^2$, an integral operator with kernel:

$$g_\mu(x,y) = \mu^2|x-y|\exp\left[-\tfrac{1}{2}(x^2+y^2) - \mu(\mu-1)(x-y)^2\right] \tag{1}$$

$$= \mu^2|x-y|\exp\left[-2(\mu-\tfrac{1}{2})^2(x^2+y^2) - \mu(1-\mu)(x+y)^2\right] \tag{1'}$$

The Rayleigh equation then reads in suitably chosen variables:

$$\partial_t u(t,x) = (Z - G_\mu)u(t,x) \tag{*}$$

(see Ref. 2, Section 2, for a derivation of this). So we need to study the spectrum of the operator $Z - G_\mu : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ for $\mu \in (1/2, \infty)$, The region $\mu > 1$ ($\mu < 1$) is then called the Rayleigh (Lorentz) regime; the form (1′) for G_μ will turn out to be useful for studying the Lorentz regime.

Let us begin by briefly noting some properties of $Z(x)$. It clearly is a C^∞ function and $Z(x)|_{x>0}$ is strictly monotonic since $Z'(x) = 2\,\mathrm{erf}(x)$. Its spectrum as an operator in L^2 is thus absolutely continuous in $(1, \infty)$ with no gaps and by the monotonicity it is easy to calculate explicitly the

Radon–Nikodym derivative of the measure $d\mu_f(\lambda)$ in the spectral resolution $(f, Zf) = \int_1^\infty \lambda d\mu_f(\lambda)$ (however, in this paper we shall have no occasion to make use of this).

Now G_μ clearly is Hilbert–Schmidt with norm $\|G_\mu\|_{\mathrm{HS}}^2 = \pi\gamma^3\mu^4$. It then follows from standard results that $Z - G_\mu$, which by its very construction is a positive operator, must have discrete spectrum in $[0, 1)$ with at most the one accumulation point 1; in this special case, however, there is no accumulation point at all.(2) However, the question whether the perturbed operator has any discrete eigenvalues embedded in its continuous spectrum or worse, whether there is in fact any continuous spectrum for a given μ remains open, since a Hilbert–Schmidt perturbation can do all kinds of nasty things to the spectrum of the unperturbed operator (Ref. 4, Theorem X.2.1). The most straightforward way of tackling this problem consists in proving that the perturbation is trace class since we know that trace-class perturbations can do nothing to the absolutely continuous spectrum (Ref. 4, Theorem X.4.4). We shall prove it in the next section (the proof is somewhat nontrivial for $\mu \leqslant 1$)—thereby showing that for all $\mu > 1/2$ there is an absolutely continuous spectrum in $[1, \infty)$.

Next we know that $Z - G_\mu$ has a ground-state (eigenvalue 0), namely,

$$N_\mu(x) = \left(\frac{2\mu - 1}{\pi}\right)^{1/4} \exp\left[-(\mu - 1/2)x^2\right].$$

whose existence stems directly from the physics and whose uniqueness mathematically is a direct consequence of the fact that G_μ is a positivity preserving operator.(5) The next thing to do is thus to find out how many discrete eigenvalues there are for a given μ and what their multiplicities are. Of this program we shall answer only one qualitative question proving the absence of discrete eigenvalues other than the ground-state value for a whole interval $\mu_1 < 1 < \mu_2$; this was conjectured in Ref. 2, where also a nonrigorous argument was given. That the conjecture is true for $\mu = 1$—the only case where a complete solution is known—is elementary and will be rederived below. Let us now prove some preliminary results. Consider the problem stated above. To show that the discretum is empty except for the ground state we must show that $(f, (Z - G_\mu)f) \geqslant \|f\|_2^2$ for all $f \in L^2(\mathbb{R}) \cap N_\mu^\perp$ so that we will have to estimate the matrix elements $(f, G_\mu f)$ by $(f, (Z - 1)f)$. For this we need a lower bound in closed form—if possible by a function easily manipulated—for the quantity $Z(x) - 1$. This we do in the following lemma.

Lemma 1. For $p \geqslant 1/6$ we have $Z(x) - 1 \geqslant x^2 e^{-px^2}$ for all $x \in \mathbb{R}$.

Proof. By symmetry we need only consider the range $x > 0$. Expanding everything in power series we get

$$T_p(x) := Z(x) - 1 - x^2 e^{-px^2} = (p - 1/6)x^4 + (1/30 - p^2/2)x^6 + \cdots$$

showing that for x sufficiently near the origin the left-hand side (l.h.s.) is positive for $p > 1/6$. Thus it is sufficient to show that the derivative of the l.h.s. which reads $2[\operatorname{erf}(x) - xe^{-px^2} + px^3e^{-px^2}]$ is positive for all $x > 0$. Since it is easily seen to be positive for very large and very small x we need only show that it is either monotone increasing or has just one extremum in $x > 0$. This in turn will be the case iff $\frac{1}{2}e^{px^2}[T_p(x)]_{xx} = e^{(p-1)x^2} - 1 + 5px^2 - 2p^2x^4$ is either everywhere positive or has exactly one zero; for $p > 1/6$ it clearly has at least one so that $[T_p(x)]_x$ cannot be monotonic. The latter will be the case iff there is a single maximum, i.e., exactly one zero of $2(p-1)e^{(p-1)x^2} + 10p - 8p^2x^2$ in $x > 0$. It then is enough to show that $4(p-1)^2e^{(p-1)x^2} - 16p^2$ is either $\leqslant 0$ for all $x > 0$ or has exactly one zero. The first case obtains for $p \geqslant 1/3$, the second case for $1/6 < p < 1/3$. Arguing backwards we get the desired result for $p > 1/6$ and thus also for $p = 1/6$ by continuity.

Lemma 2. Let P denote the orthogonal projection onto the subspace $\{e^{-x^2/2}\}^{\perp}$ of $L^2(\mathbb{R})$. Then PG_1P is negative definite.

Proof. Let $f \in \{e^{-x^2/2}\}^{\perp}$; then $e^{-x^2/2}f(x)$ is the derivative $F'(x)$ of an L^2 function $F(x)$. Integration by parts and use of the formula $\partial_x\partial_y|x - y| = -2\delta(x-y)$ yields $(f, G_1F) = -2\|F\|_2^2$.

Corollary. G_1 has only one positive eigenvalue.

Proof. Suppose there are two orthogonal, real, normalized eigenfunctions g_1, g_2 for G_1 with positive eigenvalues λ_1, λ_2. Then the two-dimensional subspace span (g_y, g_2) must contain a nonzero function $h(x) = \alpha g_1 + \beta g_2 \in \{e^{-x^2/2}\}^{\perp}$ and α, $\beta \in \mathbb{R}$. But then

$$(h, G_1h) = \alpha^2\lambda_1\|g_1\|_2^2 + \beta^2\lambda_2\|g_2\|_2^2 > 0$$

a contradiction.

Remark. From the lemma it immediately follows that the ground state is the only discrete eigenfunction in $[0,1)$ for $Z - G_1$. The corollary immediately leads to the interesting question whether G_μ has finitely or infinitely many eigenfunctions with positive eigenvalue for $\mu \neq 1$. In the first case one would get an upper bound for the number of discrete eigenfunctions of $Z - G_\mu$ from consideration of G_μ alone.

3. THE PERTURBATION IS TRACE CLASS FOR ALL VALUES OF μ

Theorem 1. G_μ is trace class for all $\mu \in (1/2, \infty)$.

Proof. We shall have to consider the three cases $\mu > 1$, $\mu < 1$, $\mu = 1$ separately.

(1) Let $\mu > 1$. Take the second distributional derivative of the function $|x|e^{-\alpha x^2}$—where from now on we shall abbreviate and set $\alpha = \mu(\mu - 1)$—to get

$$2\delta(x) - 6\alpha|x|e^{-\alpha x^2} + 4\alpha^2|x|^3 e^{-\alpha x^2}$$

From this it follows that the Fourier transform $\tilde{g}_\alpha(p)$ of $|x|e^{-\alpha x^2}$ is bounded by p^{-2}. $M(\alpha), M(\alpha) \in \mathbb{R}$. Define functions

$$\tilde{g}_1^{(\alpha)}(p) := |\tilde{g}_\alpha(p)|^{1/2}; \qquad \tilde{g}_2^{(\alpha)}(p) := \operatorname{sign}[\tilde{g}_\alpha(p)]\, \tilde{g}_1^{(\alpha)}(p)$$

By the preceding argument both functions are in $L^2(\mathbb{R})$; denoting by $g_1^{(\alpha)}(x)$, $g_2^{(\alpha)}(x)$ their inverse Fourier transforms we thus get that both kernels $e^{-x^2/2}g_1^{(\alpha)}(x-y)$; $g_2^{(\alpha)}(x-y)e^{-y^2/2}$ define Hilbert–Schmidt operators. Since their convolution product is proportional to $g_\mu(x, y)$ the latter defines a trace-class operator.

(2) The previous method clearly does not work in the Lorentz regime. So for $\mu < 1$ we try to find two HS operators whose product has the same growth as $g_\mu(x, y)$. From the formula

$$\int_{-\infty}^{\infty} |x-y| e^{-y^2/2}\, dy = Z(x)$$

we guess that kernels of the form

$$K_1; = e^{-r_1x^2 - \alpha(x-y)^2}|qx + py|; \qquad K^2(x, y) := e^{-r_2y^2 - \beta(x+y)^2}$$

with α, $\beta, r_1, r_2 > 0, p, q \in \mathbb{R}$, might do the job. The product kernel becomes

$$K_1 \circ K_2(x,z) = \frac{p}{\alpha+\beta}\exp\left[-(r_1+\alpha)x^2 - (r_2+\beta)z^2 + \frac{(\alpha x - \beta z)^2}{\alpha+\beta}\right]$$

$$\times \int_{-\infty}^{\infty}\left| t + \frac{p\alpha + q(\alpha+\beta)}{p(\alpha+\beta)^{1/2}}x - \frac{\beta}{(\alpha+\beta)^{1/2}}z\right| e^{-t^2}\,dt$$

and we see that in order to have the integral on the r.h.s. a function of $x - z$ we need

$$\frac{p\alpha + q(\alpha+\beta)}{p(\alpha+\beta)^{1/2}} = \frac{\beta}{(\alpha+\beta)^{1/2}} \Leftrightarrow \frac{q}{p} = \frac{\beta-\alpha}{\beta+\alpha}$$

Fixing tentatively $p = \alpha + \beta$, $q = \beta - \alpha$ we get for the product kernel

$$K_1 \circ K_2(x, y) = Z\left(\frac{\beta}{(\alpha+\beta)^{1/2}}(x-z)\right)\exp$$

$$\times\left[-\frac{\alpha\beta}{\alpha+\beta}(x+z)^2 - r_1x^2 - r_2z^2\right]$$

We now set $r_1 = r_2 = 2s^2, \alpha\beta/(\alpha+\beta) = \mu(1-\mu)$; $\beta/(\alpha+\beta)^{1/2} = \pi^{-1/2}$ [this is easily seen to be possible with α, $\beta > 0$ for all $\mu \in (1/2, 1)$], and it follows that the kernel

$$\exp\left[-2s^2(x^2+y^2) - \mu(1-\mu)(x+y)^2\right] \cdot Z\left(\pi^{-1/2}(x-z)\right)$$

defines a trace-class operator. Consider now the difference $G_\mu - K_1 \circ K_2$; it has a kernel of the form $\exp[-2s^2(x^2+y^2)]\varphi(x-y)\varphi(x+y)$ with $\varphi(\eta) = |\eta| - \pi^{-1/2}Z(\eta); \psi(\theta) = e^{-\mu(1-\mu)\theta^2}$.

Now we write $\exp[-\mu(1-\mu)(x+y)^2] = \exp[\mu(1-\mu)(x-y)^2 - 2\mu(1-\mu)(x^2+y^2)]$ so that the kernel of $G_\mu - K_1 \circ K_2$ actually has the form

$$\exp\left[-\sigma_\mu(x^2+y^2)\right]F_\mu(x-y) \quad \text{with} \quad F_\mu(z) = -e^{\mu(1-\mu)z^2}\left[Z\left(\frac{z}{\sqrt{\pi}}\right) - |z|\right]$$

Thus it only remains to show that $\tilde{F}_\mu(p) \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ because then we can apply the arguments of part one to show that the difference in question is trace class, too, which makes G_μ trace class as required.

However, for $x > \sqrt{\pi}$ we have

$$\left|Z\left(\frac{x}{\sqrt{\pi}}\right) - x\right| \leqslant e^{-x^2/\pi} + \frac{2x}{\sqrt{\pi}}\int_{x/\sqrt{\pi}}^{\infty} e^{-t^2}\,dt < e^{-x^2/\pi} + \frac{2x}{\sqrt{\pi}}\int_{x/\sqrt{\pi}}^{\infty} te^{-t^2}\,dt$$
$$= \left(1 + \frac{x}{\sqrt{\pi}}\right)e^{-x^2/\pi}$$

Since for $\mu \in (1/2, 1)$ we have $\mu(1-\mu) < 1/4$ we see that $F_\mu(z)$ is falling off exponentially and the theorem holds in the Lorentz regime.

(3) Neither method works for $\mu = 1$. However, from Lemma 2 we see that all we have to do is to find a suitable complete orthonormal sequence of functions in $L^2(\mathbb{R}) \cap \{e^{-x^2/2}\}^\perp, \{\varphi_n(x)\}_{n\in\mathbb{N}}$, say, and to show that

$$\sum_{n=1}^{\infty} (\varphi_n, PG_1P\varphi_n) = \sum_{n=1}^{\infty} (\varphi_n, G_1\varphi_n)$$

is finite because if PG_1P is trace class, G_1 is, too, since their difference is a degenerate operator. A suitable system of functions is readily found, namely, the Hermite functions:

$$\varphi_n(x) = \left(\pi^{1/2}2^n n!\right)^{-1/2} e^{x^2/2}\left(\partial_x^n e^{-x^2}\right), \qquad n \geqslant 1$$

By Lemma 2 we get

$$(\varphi_n, G_1\varphi_n) = -2\left(\pi^{1/2}2^n n!\right)^{-1}\|\partial_x^{n-1}e^{-x^2}\|_2^2$$

which after Fourier transformation yields

$$-(2\pi)^{-1/2}(n!)^{-1}\Gamma\left(\frac{2n-1}{2}\right) =: -a_n$$

To show that $\sum_1^\infty a_n < \infty$ we compute

$$\frac{a_n}{a_{n+1}} = \frac{n+1}{(2n-1)/2} = \frac{2n+2}{2n-1} = 1 + \frac{3/2}{n-1/2} \geqslant 1 + \frac{3/2}{n}.$$

Using now Kummer's criterion for convergence[6] with $c = 0$, $\alpha = 1/2$ we get the assertion and the theorem is proved.

Remark. Knowing now that G_μ is trace class we find that $\mathrm{Tr}(G_\mu) = 0$ for all $\mu \in (\frac{1}{2}, \infty)$ (Ref. 4, Example X.1.18). The method of proof also yields an upper bound for the trace norm of G_μ, but having no use for it we shall not give it.

4. THE DISCRETE SPECTRUM NEAR $\mu = 1$

This section is entirely devoted to the proof of the following theorem.

Theorem 2. There exist $\mu_1 < 1 < \mu_2$ such that for $\mu \in (\mu_1, \mu_2)$ and $f \in N_\mu^\perp$ we have $(f, (Z - G_\mu)f) \geqslant \|f\|_2^2$, i.e., the ground state is the only discrete eigenstate of $Z - G_\mu$ for such μ.

Proof. Since N_μ is even it turns out to be convenient to treat even and odd functions separately. For f real we write

$$(f, G_\mu f) = \mu^2 \int_{-\infty}^{\infty}\int f(x) e^{-(1/2+\alpha)x^2} |x-y| \cosh(2\alpha xy) f(y) e^{-(1/2+\alpha)y^2}\, dx\, dy$$

$$+ \mu^2 \int_{-\infty}^{\infty}\int f(x) e^{-(1/2+\alpha)x^2} |x-y| \sinh(2\alpha xy) f(y) e^{-(1/2+\alpha)y^2}\, dx\, dy \qquad (2)$$

For f odd (even) we expand $\cosh(2\alpha xy)$ [$\sinh(2\alpha xy)$] and crudely estimate setting $\varphi_\alpha(x) := f(x)\exp[-(\frac{1}{2} + \alpha)x^2]$

$$\left|\int\int \varphi_\alpha(x) x^n |x-y| \varphi_\alpha(y) y^n\, dx\, dy\right|$$

$$\leqslant 2\int |\varphi_\alpha(x)| x^{n+1}\, dx \int |\varphi_\alpha(y) y^n|\, dy$$

$$\leqslant 2\|f\|_2^2 \left[\int x^{2n+2} e^{-(1+2\alpha)x^2}\, dx \int x^{2n} 2 e^{-(1+2\alpha)x^2}\, dx\right]$$

$$= 2\|f\|_2^2 \Gamma\left(\frac{2n+1}{2}\right)\left(\frac{2n+1}{2}\right)^{1/2} (1+2\alpha)^{-(n+1)}$$

$$\leqslant M(n!)(1+2\alpha)^{-(n+1)}$$

Thus we see that for f odd (even) the first (second) summand on the r.h.s. of (2) can be evaluated term by term for all $\alpha > -1/4$ and by Lemma 2 gives a negative contribution for all $\alpha > -1/4$ if f is odd and for $\alpha > 0$ if f is even. The case "f even and $\alpha < 0$" needs a separate argument.

In order to rid ourselves of various complications it is convenient to reduce the respective remainders first to integration over the first quadrant and then by symmetry to integration over the wedge-shaped region $0 \leqslant y \leqslant x$. For f odd this gives

$$8\mu^2 \int_0^\infty dx\, x\varphi_\alpha(x) \int_0^x \sinh(2\alpha xy)\varphi_\alpha(y)\, dy$$

whereas for f even we get

$$8\mu^2 \int_0^\infty dx\, x\varphi_\alpha(x) \int_0^x \cosh(2\alpha xy)\varphi_\alpha(y)\, dy$$

In the first case we estimate by means of the simple formula $\sinh(x) \leqslant xe^x$, $x \geqslant 0$, and we get for $\alpha > 0$

$$\begin{aligned}
&\left|\int^\infty dx\, x\varphi_\alpha(x) \int_0^x \sinh(2\alpha xy)\varphi_\alpha(y)\, dy\right| \\
&\leqslant 2\alpha \int_0 x^2 |\varphi_\alpha(x)|\, dx \int_0^x ye^{2\alpha xy} |\varphi_\alpha(y)|\, dy \\
&\leqslant 2\alpha \int_0^\infty x^2 e^{-x^2/2} |f(x)|\, dx \int_0^x e^{-\alpha(x-y)^2} ye^{-y^2/2} |f(y)|\, dy \\
&\leqslant 2\alpha \left[\int_0^\infty x^2 e^{-2qx^2}\, dx \int_0^\infty e^{-2qx^2}\, dx\right]^{1/2} \\
&\qquad \times \int_0^\infty x^2 e^{-2(1/2-q)x^2} f^2(x)\, dx, \qquad q \in (0, 1/2)
\end{aligned}$$

and analogously for $\alpha < 0$:

$$\begin{aligned}
&\left|\int_0^\infty x\varphi_\alpha(y)\, dx \int_0^x \sinh(2\alpha xy)\varphi_\alpha(y)\, dy\right| \\
&\leqslant 2|\alpha| \int_0^\infty x^2 e^{-(1/2+2\alpha)x^2} |f(x)|\, dx \int_0^x e^{-|\alpha|(x-y)^2} ye^{-(1/2+2\alpha)y^2} |f(y)|\, dy \\
&\leqslant 2|\alpha| \frac{\pi}{16q^2} \int_0^\infty x^2 e^{-2(1/2+2\alpha-q)x^2} f^2(x)\, dx, \qquad q \in (0, \tfrac{1}{2} + 2)
\end{aligned}$$

Since for α in a neighborhood of zero we can fix q this estimate meets all our requirements. It also takes care of the case f even and $\alpha < 0$ because then the second term on the r.h.s. reads

$$-8\mu^2 \int_0^\infty dx\, \varphi_\alpha(x) \int_0^x y \sinh(2\alpha xy)\varphi_\alpha(y)\, dy$$

In a similar way (with different constants, of course) we can estimate the expression

$$\int_0^\infty dx\, x\varphi_\alpha(x) \int_0^x [\cosh(2\alpha xy) - 1]\varphi_\alpha(y)\, dy$$

for f even. The only problem then remaining is presented by the term

$$\int_0^\infty dx\, x\varphi_\alpha(x)\int_0^x \varphi_\alpha(y)\, dy$$

It is here that the condition $f \in N_\mu^\perp$ enters in a very specific way. We write $K(x) := \int_0^x \varphi_\alpha(y)\, dy$ and define $K(\infty) := \int_0^\infty \varphi_\alpha(y)\, dy$, a finite number and we find

$$\int_0^\infty x\varphi_\alpha(x)k(x)\, dx = -\frac{1}{2}\int_0^\infty [K(x) - K(\infty)]^2 dx + K(\infty)\int_0^\infty x\varphi_\alpha(x)\, dx$$

the first term on the r.h.s. being finite since $K(x) - K(\infty)$ is a rapidly decreasing function. In order to estimate the second term we use the following simple inequality: for $b > a > 0, x > 0$ we have

$$e^{-ax^2} - e^{-bx^2} \leqslant qxe^{-2x^2}$$

with

$$q = [2(b-a)/e]^{1/2}.$$

(Proof: the assertion is equivalent to $qx + e^{-(b-a)x^2} - 1 \geqslant 0$; this holds if $q - 2x(b-a)e^{-(b-a)x^2} \geqslant 0$ for all $x > 0$; and therefore if the supremum of $2x(b-a)e^{-(b-a)x^2}$—which is $[2(b-a)/e]^{1/2}$—is not larger than q.)

Now setting $a := \mu - 1/2$, $b := \alpha + 1/2$ the assumption $f \in N_\mu^\perp$ yields

$$|K(\infty)| = \left|\int_0^\infty [e^{-ax^2} - e^{-bx^2}] f(x)\, dx\right| > \left(\frac{2}{e}\right)^{1/2} |\mu - 1| \int_0^\infty xe^{-ax^2}|f(x)|\, dx$$

$$\leqslant \left(\frac{2}{e}\right)^{1/2} |\mu - 1| \left[\frac{1}{2}(f, x^2e^{-ax^2}f)_2 \int_0^\infty e^{-ax^2} dx\right]^{1/2}$$

and even easier for the other factor

$$\left|\int_0^\infty xe^{-bx^2}f(x)\, dx\right| \leqslant \int_0^\infty xe^{-ax^2}|f(x)|\, dx$$

which gives

$$\left|K(\infty)\int_0^\infty x\varphi_\alpha(x)\, dx\right| \leqslant \frac{|\mu - 1|}{(2e)^{1/2}}\left(\frac{\pi}{2\mu - 1}\right)^{1/2}(f, x^2e^{-ax^2}f)_2$$

The contribution from this term in modulus is thus not larger than

$$4\mu^2|\mu - 1|\left[\frac{\pi}{2e(2\mu - 1)}\right]^{1/2}(f, x^2e^{-ax^2}f)_2$$

Putting everything together it is now clear that in a suitable neighborhood of $\alpha = 0$ we have the inequality of the theorem.

Remark. We shall not give a numerical value for μ_1 and μ_2 since it is clear from the proof that this value would be nowhere near the true values.

However, there are innumerable ways of extracting negative parts from $(f, G_\mu f)$ so with an appropriate split one should be able to do much better than we did here by canceling some of the positive (i.e., bad) contributions against some of the negative ones. The problem of getting numerically satisfactory bounds for μ_1, μ_2 or, better still, convergent expansions for these values will be taken up in a future paper.

5. THE RAYLEIGH AND LORENTZ LIMITS

We ask: to which limit operators and in what topological sense does $Z - G_\mu$ converge in the case $\mu \to \infty$ (the Rayleigh limit) and $\mu \to 1/2$ (the Lorentz limit)? Let us remark here that these limit operators (if they exist) are not of direct physical interest as generators of interesting processes; but the structure of their spectra tells us what the spectrum of $Z - G_\mu$ looks like —qualitatively—for either $\mu \gg 1$ or $\mu - 1/2 \ll 1$. Since we are at present only concerned with the qualitative aspect of the spectrum this abuse of language seems to be justified. The first case is trivial since $\mu^2 e^{-\alpha(x-y)^2}$ converges to a ∂ kernel if $\mu \to \infty$ and the $\{G_\mu\}_{\mu>1}$ are a uniformly bounded family of operators so $Z - G_\mu$ converges strongly in the generalized sense to the multiplication operator $2x\ \mathrm{erf}(x)$ (Ref. 4, Chap. 8). Clearly $2x\,\mathrm{erf}(x)$ has absolutely continuous spectrum in $(0, \infty)$ with no gap; so from the operator theoretic point of view there remains only the problem of determining the "rate of convergence" of the spectra of $Z - G_\mu$, i.e., how fast do the discrete eigenvalues fill out the interval $(0, 1)$ (Ref. 4, Theorem VIII.1.15)?

However, the Lorentz limit, which does not seem to have attracted much attention so far, turns out to be a much more subtle affair; so far we have only very general results which we summarize in the following theorem.

Theorem 3. Denote by $G_{1/2}$ the operator defined by the kernel

$$g_{1/2}(x, y) = \tfrac{1}{4}|x - y| e^{-(x+y)^2/4}$$

which is an unbounded, symmetric operator on some domain, $\mathcal{S}(\mathbb{R})$ say. One then has an operator bound for $f \in \mathcal{S}$:

$$\|G_{1/2} f\|^2 \leqslant A\|f\|^2 + \|Zf\|^2$$

so for the closure of $G_{1/2}$ (denoted by $\hat{G}_{1/2}$) we have $\mathfrak{D}(\hat{G}_{1/2}) \supset \mathfrak{D}(Z)$ and $Z - \hat{G}_{1/2}$ is essentially self-adjoint on every core for Z. Furthermore for $f \in \mathcal{S}$ we have

$$s - \lim_{\mu \to 1/2} (Z - G_\mu) f = (Z - \hat{G}_{1/2}) f$$

and so here also we have strong convergence in the generalized sense (Ref. 4, Corollary VIII.1.6).

Proof. We first compute the iteration kernel of $G_{1/2}^2$ which is

$$h(x,z) = \frac{1}{16} e^{-(x-z)^2/8} \int_{-\infty}^{\infty} |[y-(x+z)]^2 - \tfrac{1}{4}(x-z)^2| e^{-y^2/2} dy$$

then for any function in $\mathcal{S}(\mathbb{R})$ we get

$$\begin{aligned}(f, G_{1/2}^2 f) &\leqslant \frac{1}{16} \int_{-\infty}^{\infty} \int dx\, dz\, |f(x)f(z)|\, e^{-(x-z)^2/8} \int_{-\infty}^{\infty} \\ &\quad \times |[y-(x+z)]^2 - \tfrac{1}{4}(x-z)^2| e^{-y^2/2} dy \\ &\leqslant \frac{(2\pi)^{1/2}}{16} \int\int dx\, dz\, |f(x)f(z)| e^{-(x-z)^2/8} \\ &\quad \times \left[\frac{(x-z)^2}{4} + (x+z)^2 + 1 \right] \\ &\leqslant \frac{(2\pi)^{1/2}}{16} \int\int dx\, dz\, |f(x)f(z)| e^{-(x-z)^2/8} \\ &\quad \times \left[1 + \frac{5}{4}(x-z)^2 + 4|xz| \right]\end{aligned}$$

If therefore we denote by U_1 the operator defined by the kernel

$$e^{-(x-z)^2/8}\left[1 + \tfrac{5}{4}(x-z)^2\right] \qquad (U_1 \text{ bounded})$$

and by U_2 the operator defined by the kernel $|xz|e^{-(x-z)^2/8}$ we get

$$\begin{aligned}(f, G_{1/2}^2 f) &\leqslant \frac{(2\pi)^{1/2}}{16}(|f|, U_1|f|) + \frac{(2\pi)^{1/2}}{4}(|f|, U_2|f|) \\ &\leqslant \frac{(2\pi)^{1/2}}{16} \|U_1\|\, \|f\|_2^2 + \frac{(2\pi)^{1/2}(8\pi)^{1/2}}{4} \|(x \mid f(x))\|_2^2\end{aligned}$$

it follows that $\|G_{1/2}f\|_2^2 \leqslant \|f\|_2^2 + \|Zf\|_2^2$ the required operator bound (Ref. 4, Theorem V.4.6).

The second part of the theorem is easily proved by inserting the multiplication operator $(1+x^2)^{-2}(1+x^2)^2$ between G_μ and $f \in \mathcal{S}$ and noting that the family of operators $\{G_\mu(1+y^2)^{-2}\}_{\mu\in[1/2,1)}$ is a family of uniformly bounded operators which strongly converges for $\mu \to 1/2$.

A final remark: it has been conjectured that the spectrum of $Z - G_\mu$ should be the set $\{0\} \cup [1,\infty)$ for all $\mu \in (\frac{1}{2}, 1)$. The previous result shows that this cannot be true. For, suppose it were, by Ref. 4, Theorem VIII.1.14 we would have $\mathrm{Sp}(\overline{Z - G_{1/2}}) \subset \{0\} \cup [1,\infty)$, where $\overline{Z - G_{1/2}}$ denotes the self-adjoint closure of $Z - \hat{G}_{1/2}$. If now ψ were an eigenvector of $\overline{Z - G_{1/2}}$ with eigenvalue 0 we would—by the strong convergence of the resolvents $(Z - G_\mu + 1)^{-1}$ to $(\overline{Z - G_{1/2}} + 1)^{-1}$—find that

$$\|N_\mu - \psi\| \to 0 \qquad \text{for } \mu \to 1/2$$

So there is no such eigenvector and therefore—if the assumption were true —the spectrum of $\overline{Z - G_{1/2}}$ would actually be in $[1, \infty)$. Thus, however, it is not because we have by direct computation

$$\left(N_\mu, \overline{Z - G_{1/2}} N_\mu\right) = \left[(2\mu - 1)/2\mu\right]^{1/2}$$

converging to zero for $\mu \to 1/2$. So something has to happen with the spectra of the $Z - G_\mu$ for $\mu \to 1/2$ although what this something is we do not yet know.

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