

8

Spectral Theory

Introduction

This chapter is devoted to the spectral theory of self-adjoint, differential operators. We cover a number of different topics, beginning in §1 with a proof of the spectral theorem. It was an arbitrary choice to put that material here, rather than in Appendix A, on functional analysis. The main motivation for putting it here is to begin a line of reasoning that will be continued in subsequent sections, using the great power of studying unitary groups as a tool in spectral theory. After we show how easily this study leads to a proof of the spectral theorem in §1, in later sections we use it in various ways: as a tool to establish self-adjointness, as a tool for obtaining specific formulas, including basic identities among special functions, and in other capacities.

Sections 2 and 3 deal with some general questions in spectral theory, such as when does a differential operator define a self-adjoint operator, when does it have a compact resolvent, and what asymptotic properties does its spectrum have? We tackle the latter question, for the Laplace operator Δ , by examining the asymptotic behavior of the trace of the solution operator $e^{t\Delta}$ for the heat equation, showing that

$$(0.1) \quad \text{Tr } e^{t\Delta} = (4\pi t)^{-n/2} \text{ vol } \Omega + o(t^{-n/2}), \quad t \searrow 0,$$

when Ω is either a compact Riemannian manifold or a bounded domain in \mathbb{R}^n (and has the Dirichlet boundary condition). Using techniques developed in §13 of Chap. 7, we could extend (0.1) to general compact Riemannian manifolds with smooth boundary and to other boundary conditions, such as the Neumann boundary condition. We use instead a different method here in §3, one that works without any regularity hypotheses on $\partial\Omega$. In such generality, (0.1) does not necessarily hold for the Neumann boundary problem.

The study of (0.1) and refinements got a big push from [Kac]. As pursued in [MS], it led to developments that we will discuss in Chap. 10. The problem of to what extent a Riemannian manifold is determined by the spectrum of its Laplace operator has led to much work, which we do not include here. Some is discussed

in [Ber, Br, BGM], and [Cha]. We mention particularly some distinct regions in \mathbb{R}^2 whose Laplace operators have the same spectra, given in [GWW].

We have not included general results on the spectral behavior of Δ obtained via geometrical optics and its refinement, the theory of Fourier integral operators. Results of this nature can be found in Volume 3 of [Ho], in [Shu], and in Chap. 12 of [T1].

Sections 4–7 are devoted to specific examples. In §4 we study the Laplace operator on the unit spheres S^n . We specify precisely the spectrum of Δ and discuss explicit formulas for certain functions of Δ , particularly

$$(0.2) \quad A^{-1} \sin tA, \quad A = \left(-\Delta + \frac{K}{4}(n-1)^2 \right)^{1/2}.$$

with $K = 1$, the sectional curvature of S^n . In §5 we obtain an explicit formula for (0.2), with $K = -1$, on hyperbolic space. In §6 we study the spectral theory of the harmonic oscillator

$$(0.3) \quad H = -\Delta + |x|^2.$$

We obtain an explicit formula for e^{-tH} , an analogue of which will be useful in Chap. 10. In §8 we study the operator

$$(0.4) \quad H = -\Delta - K|x|^{-1}$$

on \mathbb{R}^3 , obtaining in particular all the eigenvalues of this operator. This operator arises in the simplest quantum mechanical model of the hydrogen atom. In §9 we study the Laplace operator on a cone. Studies done in these sections bring in a number of special functions, including Legendre functions, Bessel functions, and hypergeometric functions. We have included two auxiliary problem sets, one on confluent hypergeometric functions and one on hypergeometric functions.

1. The spectral theorem

Appendix A contains a proof of the spectral theorem for a compact, self-adjoint operator A on a Hilbert space H . In that case, H has an orthonormal basis $\{u_j\}$ such that $Au_j = \lambda_j u_j$, λ_j being real numbers having only 0 as an accumulation point. The vectors u_j are eigenvectors.

A general bounded, self-adjoint operator A may not have any eigenvectors, and the statement of the spectral theorem is somewhat more subtle. The following is a useful version.

Theorem 1.1. *If A is a bounded, self-adjoint operator on a separable Hilbert space H , then there is a σ -compact space Ω , a Borel measure μ , a unitary map*

$$(1.1) \quad W : L^2(\Omega, d\mu) \longrightarrow H,$$

and a real-valued function $a \in L^\infty(\Omega, d\mu)$ such that

$$(1.2) \quad W^{-1}AWf(x) = a(x)f(x), \quad f \in L^2(\Omega, d\mu).$$

Note that when A is compact, the eigenvector decomposition above yields (1.1) and (1.2) with (Ω, μ) a purely atomic measure space. Later in this section we will extend Theorem 1.1 to the case of unbounded, self-adjoint operators.

In order to prove Theorem 1.1, we will work with the operators

$$(1.3) \quad U(t) = e^{itA},$$

defined by the power-series expansion

$$(1.4) \quad e^{itA} = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} A^n.$$

This is a special case of a construction made in §4 of Chap. 1. $U(t)$ is uniquely characterized as the solution to the differential equation

$$(1.5) \quad \frac{d}{dt}U(t) = iAU(t), \quad U(0) = I.$$

We have the group property

$$(1.6) \quad U(s+t) = U(s)U(t),$$

which follows since both sides satisfy the ODE $(d/ds)Z(s) = iAZ(s)$, $Z(0) = U(t)$. If $A = A^*$, then applying the adjoint to (1.4) gives

$$(1.7) \quad U(t)^* = U(-t),$$

which is the inverse of $U(t)$ in view of (1.6). Thus $\{U(t) : t \in \mathbb{R}\}$ is a group of unitary operators.

For a given $v \in H$, let H_v be the closed linear span of $\{U(t)v : t \in \mathbb{R}\}$; we say H_v is the cyclic space generated by v . We say v is a cyclic vector for H if $H = H_v$. If H_v is not all of H , note that H_v^\perp is invariant under $U(t)$, that is, $U(t)H_v^\perp \subset H_v^\perp$ for all t , since for a linear subspace V of H , generally

$$(1.8) \quad U(t)V \subset V \implies U(t)^*V^\perp \subset V^\perp.$$

Using this observation, we can prove the next result.

Lemma 1.2. *If $U(t)$ is a unitary group on a separable Hilbert space H , then H is an orthogonal direct sum of cyclic subspaces.*

Proof. Let $\{w_j\}$ be a countable, dense subset of H . Take $v_1 = w_1$ and $H_1 = H_{v_1}$. If $H_1 \neq H$, let v_2 be the first nonzero element $P_1 w_j$, $j \geq 2$, where P_1 is the orthogonal projection of H onto H_1^\perp , and let $H_2 = H_{v_2}$. Continue.

In view of this, Theorem 1.1 is a consequence of the following:

Proposition 1.3. *If $U(t)$ is a strongly continuous, unitary group on H , having a cyclic vector v , then we can take $\Omega = \mathbb{R}$, and there exists a positive Borel measure μ on \mathbb{R} and a unitary map $W : L^2(\mathbb{R}, d\mu) \rightarrow H$ such that*

$$(1.9) \quad W^{-1}U(t)W f(x) = e^{itx} f(x), \quad f \in L^2(\mathbb{R}, d\mu).$$

The measure μ on \mathbb{R} will be the Fourier transform

$$(1.10) \quad \mu = \hat{\zeta},$$

where

$$(1.11) \quad \zeta(t) = (2\pi)^{-1/2} (e^{itA} v, v).$$

It is not clear a priori that (1.10) defines a measure; since $\zeta \in L^\infty(\mathbb{R})$, we see that μ is a tempered distribution. We will show that μ is indeed a positive measure during the course of our argument. As for the map W , we first define

$$(1.12) \quad W : \mathcal{S}(\mathbb{R}) \longrightarrow H,$$

where $\mathcal{S}(\mathbb{R})$ is the Schwartz space of rapidly decreasing functions, by

$$(1.13) \quad W(f) = f(A)v,$$

where we define the operator $f(A)$ by the formula

$$(1.14) \quad f(A) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \hat{f}(t) e^{itA} dt.$$

The reason for this notation will become apparent shortly; see (1.20). Making use of (1.10), we have

$$\begin{aligned} (f(A)v, g(A)v) &= (2\pi)^{-1} \left(\int \hat{f}(s) e^{isA} v ds, \int \hat{g}(t) e^{itA} v dt \right) \\ &= (2\pi)^{-1} \iint \hat{f}(s) \overline{\hat{g}(t)} (e^{i(s-t)A} v, v) ds dt \\ (1.15) \quad &= (2\pi)^{-1/2} \iint \hat{f}(s) \hat{\bar{g}}(\sigma - s) \zeta(\sigma) ds d\sigma \\ &= \langle \widehat{f\bar{g}}, \zeta \rangle \\ &= \langle f\bar{g}, \mu \rangle. \end{aligned}$$

Now, if $g = f$, the left side of (1.15) is $\|f(A)v\|^2$, which is ≥ 0 . Hence

$$(1.16) \quad \langle |f|^2, \mu \rangle \geq 0, \quad \text{for all } f \in \mathcal{S}(\mathbb{R}).$$

With this, we can establish:

Lemma 1.4. *The tempered distribution μ , defined by (1.10)–(1.11), is a positive measure on \mathbb{R} .*

Proof. Apply (1.16) with $f = \sqrt{F_{s,\sigma}}$, where

$$F_{s,\sigma}(\tau) = (4\pi s)^{-1/2} e^{-(\tau-\sigma)^2/4s}, \quad s > 0, \sigma \in \mathbb{R}.$$

Note that this is a fundamental solution to the heat equation. For each $s > 0$, $F_{s,0} * \mu$ is a positive function. We saw in Chap. 3 that $F_{s,0} * \mu$ converges to μ in $\mathcal{S}'(\mathbb{R})$ as $s \rightarrow 0$, so this implies that μ is a positive measure.

Now we can finish the proof of Proposition 1.3. From (1.15) we see that W has a unique continuous extension

$$(1.17) \quad W : L^2(\mathbb{R}, d\mu) \longrightarrow H,$$

and W is an isometry. Since v is assumed to be cyclic, the range of W must be dense in H , so W must be unitary. From (1.14) it follows that if $f \in \mathcal{S}(\mathbb{R})$, then

$$(1.18) \quad e^{isA} f(A) = f_s(A), \quad \text{with } f_s(\tau) = e^{is\tau} f(\tau).$$

Hence, for $f \in \mathcal{S}(\mathbb{R})$,

$$(1.19) \quad W^{-1} e^{isA} W f = W^{-1} f_s(A) v = e^{is\tau} f(\tau).$$

Since $\mathcal{S}(\mathbb{R})$ is dense in $L^2(\mathbb{R}, d\mu)$, this gives (1.9). Thus the spectral theorem for bounded, self-adjoint operators is proved.

Given (1.9), we have from (1.14) that

$$(1.20) \quad W^{-1} f(A) W g(x) = f(x) g(x), \quad f \in \mathcal{S}(\mathbb{R}), \quad g \in L^2(\mathbb{R}, d\mu),$$

which justifies the notation $f(A)$ in (1.14).

Note that (1.9) implies

$$(1.21) \quad W^{-1} A W f(x) = x f(x), \quad f \in L^2(\mathbb{R}, d\mu),$$

since $(d/dt)U(t) = iAU(t)$. The essential supremum of x on (\mathbb{R}, μ) is equal to $\|A\|$. Thus μ has compact support in \mathbb{R} if A is bounded. If a self-adjoint operator A has the representation (1.21), one says A has *simple spectrum*. It follows from Proposition 1.3 that A has simple spectrum if and only if it has a cyclic vector.

One can generalize the results above to a k -tuple of commuting, bounded, self-adjoint operators $A = (A_1, \dots, A_k)$. In that case, for $t = (t_1, \dots, t_k) \in \mathbb{R}^k$, set

$$(1.22) \quad U(t) = e^{it \cdot A}, \quad t \cdot A = t_1 A_1 + \dots + t_k A_k.$$

The hypothesis that the A_j all commute implies $U(t) = U_1(t_1) \cdots U_k(t_k)$, where $U_j(s) = e^{isA_j}$. $U(t)$ in (1.22) continues to satisfy the properties (1.6) and (1.7); we have a k -parameter unitary group. As above, for $v \in H$, we set H_v equal to the closed linear span of $\{U(t)v : t \in \mathbb{R}^k\}$, and we say v is a cyclic vector provided $H_v = H$. Lemma 1.2 goes through in this case. Furthermore, for $f \in \mathcal{S}(\mathbb{R}^k)$, we can define

$$(1.23) \quad f(A) = (2\pi)^{-k/2} \int \hat{f}(t) e^{it \cdot A} dt,$$

and if H has a cyclic vector v , the proof of Proposition 1.3 generalizes, giving a unitary map $W : L^2(\mathbb{R}^k, d\mu) \rightarrow H$ such that

$$(1.24) \quad W^{-1}U(t)Wf(x) = e^{it \cdot x} f(x), \quad f \in L^2(\mathbb{R}^k, d\mu), \quad t \in \mathbb{R}^k.$$

Therefore, Theorem 1.1 has the following extension

Proposition 1.5. *If $A = (A_1, \dots, A_k)$ is a k -tuple of commuting, bounded, self-adjoint operators on H , there is a measure space (Ω, μ) , a unitary map $W : L^2(\Omega, d\mu) \rightarrow H$, and real-valued $a_j \in L^\infty(\Omega, d\mu)$ such that*

$$(1.25) \quad W^{-1}A_j Wf(x) = a_j(x)f(x), \quad f \in L^2(\Omega, d\mu), \quad 1 \leq j \leq k.$$

A bounded operator $B \in \mathcal{L}(H)$ is said to be normal provided B and B^* commute. Equivalently, if we set

$$(1.26) \quad A_1 = \frac{1}{2}(B + B^*), \quad A_2 = \frac{1}{2i}(B - B^*),$$

then $B = A_1 + iA_2$, and (A_1, A_2) is a 2-tuple of commuting, self-adjoint operators. Applying Proposition 1.5 and setting $b(x) = a_1(x) + ia_2(x)$, we have:

Corollary 1.6. *If $B \in \mathcal{L}(H)$ is a normal operator, there is a unitary map $W : L^2(\Omega, d\mu) \rightarrow H$ and a (complex-valued) $b \in L^\infty(\Omega, d\mu)$ such that*

$$(1.27) \quad W^{-1}BWf(x) = b(x)f(x), \quad f \in L^2(\Omega, d\mu).$$

In particular, Corollary 1.6 holds when $B = U$ is unitary. We next extend the spectral theorem to an unbounded, self-adjoint operator A on a Hilbert space H , whose domain $\mathcal{D}(A)$ is a dense linear subspace of H . This extension, due to

von Neumann, uses von Neumann's unitary trick, described in (8.18)–(8.19) of Appendix A. We recall that, for such A , the following three properties hold:

$$(1.28) \quad \begin{aligned} A \pm i : \mathcal{D}(A) &\longrightarrow H \text{ bijectively,} \\ U = (A - i)(A + i)^{-1} &\text{ is unitary on } H, \\ A = i(I + U)(I - U)^{-1}, \end{aligned}$$

where the range of $I - U = 2i(A + i)^{-1}$ is $\mathcal{D}(A)$. Applying Corollary 1.6 to $B = U$, we have the following theorem:

Theorem 1.7. *If A is an unbounded, self-adjoint operator on a separable Hilbert space H , there is a measure space (Ω, μ) , a unitary map $W : L^2(\Omega, d\mu) \rightarrow H$, and a real-valued measurable function a on Ω such that*

$$(1.29) \quad W^{-1}AWf(x) = a(x)f(x), \quad Wf \in \mathcal{D}(A).$$

In this situation, given $f \in L^2(\Omega, d\mu)$, Wf belongs to $\mathcal{D}(A)$ if and only if the right side of (1.29) belongs to $L^2(\Omega, d\mu)$.

The formula (1.29) is called the “spectral representation” of a self-adjoint operator A . Using it, we can extend the functional calculus defined by (1.14) as follows. For a Borel function $f : \mathbb{R} \rightarrow \mathbb{C}$, define $f(A)$ by

$$(1.30) \quad W^{-1}f(A)Wg(x) = f(a(x))g(x).$$

If f is a bounded Borel function, this is defined for all $g \in L^2(\Omega, d\mu)$ and provides a bounded operator $f(A)$ on H . More generally,

$$(1.31) \quad \mathcal{D}(f(A)) = \{Wg \in H : g \in L^2(\Omega, d\mu) \text{ and } f(a(x))g \in L^2(\Omega, d\mu)\}.$$

In particular, we can define e^{itA} , for unbounded, self-adjoint A , by

$$W^{-1}e^{itA}Wg = e^{ita(x)}g(x)$$

Then e^{itA} is a strongly continuous unitary group, and we have the following result, known as Stone's theorem (stated as Proposition 9.5 in Appendix A):

Proposition 1.8. *If A is self-adjoint, then iA generates a strongly continuous, unitary group, $U(t) = e^{itA}$.*

Note that Lemma 1.2 and Proposition 1.3 are proved for a strongly continuous, unitary group $U(t) = e^{itA}$, without the hypothesis that A be bounded. This yields the following analogue of (1.2):

$$(1.32) \quad W^{-1}U(t)Wf(x) = e^{ita(x)}f(x), \quad f \in L^2(\Omega, d\mu),$$

for this more general class of unitary groups. Sometimes a direct construction, such as by PDE methods, of $U(t)$ is fairly easy. In such a case, the use of $U(t)$ can be a more convenient tool than the unitary trick involving (1.28).

We say a self-adjoint operator A is positive, $A \geq 0$, provided $(Au, u) \geq 0$, for all $u \in \mathcal{D}(A)$. In terms of the spectral representation, this says we have (1.29) with $a(x) \geq 0$ on Ω . In such a case, e^{-tA} is bounded for $t \geq 0$, even for complex t with $\operatorname{Re} t \geq 0$, and also defines a strongly continuous semigroup. This proves Proposition 9.4 of Appendix A.

Given a self-adjoint operator A and a Borel set $S \subset \mathbb{R}$, define $P(S) = \chi_S(A)$, that is, using (1.29),

$$(1.33) \quad W^{-1}P(S)Wg = \chi_S(a(x))g(x), \quad g \in L^2(\Omega, d\mu),$$

where χ_S is the characteristic function of S . Then each $P(S)$ is an orthogonal projection. Also, if $S = \bigcup_{j \geq 1} S_j$ is a countable union of disjoint Borel sets S_j , then, for each $u \in H$,

$$(1.34) \quad \lim_{n \rightarrow \infty} \sum_{j=1}^n P(S_j)u = P(S)u,$$

with convergence in the H -norm. This is equivalent to the statement that

$$\sum_{j=1}^n \chi_{S_j}(a(x))g \rightarrow \chi_S(a(x))g \text{ in } L^2\text{-norm, for each } g \in L^2(\Omega, d\mu),$$

which in turn follows from Lebesgue's dominated convergence theorem. By (1.34), $P(\cdot)$ is a strongly countably additive, projection-valued measure. Then (1.30) yields

$$(1.35) \quad f(A) = \int f(\lambda) P(d\lambda).$$

$P(\cdot)$ is called the *spectral measure* of A .

One useful formula for the spectral measure is given in terms of the jump of the resolvent $R_\lambda = (\lambda - A)^{-1}$, across the real axis. We have the following

Proposition 1.9. *For bounded, continuous $f : \mathbb{R} \rightarrow \mathbb{C}$,*

$$(1.36) \quad f(A)u = \lim_{\varepsilon \searrow 0} \frac{1}{2\pi i} \int_{-\infty}^{\infty} f(\lambda) \left[(\lambda - i\varepsilon - A)^{-1} - (\lambda + i\varepsilon - A)^{-1} \right] u \, d\lambda.$$

Proof. Since $W^{-1}f(A)W$ is multiplication by $f(a(x))$, (1.36) follows from the fact that

$$(1.37) \quad \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\varepsilon f(\lambda)}{(\lambda - a(x))^2 + \varepsilon^2} d\lambda \longrightarrow f(a(x)),$$

pointwise and boundedly, as $\varepsilon \searrow 0$.

An important class of operators $f(A)$ are the fractional powers $f(A) = A^\alpha$, $\alpha \in (0, \infty)$, defined by (1.30)–(1.31), with $f(\lambda) = \lambda^\alpha$, provided $A \geq 0$. Note that if $g \in C([0, \infty))$ satisfies $g(0) = 1$, $g(\lambda) = O(\lambda^{-\alpha})$ as $\lambda \rightarrow \infty$, then, for $u \in H$,

$$(1.38) \quad u \in \mathcal{D}(A^\alpha) \iff \|A^\alpha g(\varepsilon A)u\|_H \text{ is bounded, for } \varepsilon \in (0, 1],$$

as follows easily from the characterization (1.31) and Fatou's lemma. We note that Proposition 2.2 of Chap. 4 applies to $\mathcal{D}(A^\alpha)$, describing it as an interpolation space.

We particularly want to identify $\mathcal{D}(A^{1/2})$, when A is a positive, self-adjoint operator on a Hilbert space H constructed by the Friedrichs method, as described in Proposition 8.7 of Appendix A. Recall that this arises as follows. One has a Hilbert space H_1 , a continuous injection $J : H_1 \rightarrow H$ with dense range, and one defines A by

$$(1.39) \quad (A(Ju), Jv)_H = (u, v)_{H_1},$$

with

$$(1.40) \quad \mathcal{D}(A) = \{Ju \in JH_1 \subset H : v \mapsto (u, v)_{H_1} \text{ is continuous in } Jv, \text{ in the } H\text{-norm}\}.$$

We establish the following.

Proposition 1.10. *If A is obtained by the Friedrichs extension method (1.39)–(1.40), then*

$$(1.41) \quad \mathcal{D}(A^{1/2}) = J(H_1) \subset H.$$

Proof. $\mathcal{D}(A^{1/2})$ consists of elements of H that are limits of sequences in $\mathcal{D}(A)$, in the norm $\|A^{1/2}u\|_H + \|u\|_H$. As shown in the proof of Proposition 8.7 in Appendix A, $\mathcal{D}(A) = \mathcal{R}(JJ^*)$. Now

$$(1.42) \quad \|A^{1/2}JJ^*f\|_H^2 = (AJJ^*f, JJ^*f)_H = \|J^*f\|_{H_1}^2.$$

Thus a sequence (JJ^*f_n) converges in the $\mathcal{D}(A^{1/2})$ -norm (to an element g) if and only if (J^*f_n) converges in the H_1 -norm (to an element u), in which case $g = Ju$. Since $J^* : H \rightarrow H_1$ has dense range, precisely all $u \in H_1$ arise as limits of such (J^*f_n) , so the proposition is proved.

Exercises

1. The definition (1.33) of the spectral measure $P(\cdot)$ of a self-adjoint operator A depends a priori on a choice of the spectral representation of A . Show that any two spectral representations of A yield the same spectral measure.
(Hint: For $f \in \mathcal{S}(\mathbb{R})$, $f(A)$ is well defined by (1.14), or alternatively by (1.36).)

2. Self-adjoint differential operators

In this section we present some examples of differential operators on a manifold Ω which, with appropriately specified domains, give unbounded, self-adjoint operators on $L^2(\Omega, dV)$, dV typically being the volume element determined by a Riemannian metric on Ω .

We begin with self-adjoint operators arising from the Laplacian, making use of material developed in Chap. 5. Let $\overline{\Omega}$ be a smooth, compact Riemannian manifold with boundary, or more generally the closure of an open subset Ω of a compact manifold M without boundary. Then, as shown in Chap. 5,

$$(2.1) \quad I - \Delta : H_0^1(\Omega) \longrightarrow H_0^1(\Omega)^*$$

is bijective, with inverse we denote T ; if we restrict T to $L^2(\Omega)$,

$$(2.2) \quad T : L^2(\Omega) \longrightarrow L^2(\Omega) \text{ is compact and self-adjoint.}$$

Denote by $\mathcal{R}(T)$ the image of $L^2(\Omega)$ under T . We can apply Proposition 8.2 of Appendix A to deduce the following

Proposition 2.1. *If Ω is a region in a compact Riemannian manifold M , then Δ is self-adjoint on $L^2(\Omega)$, with domain $\mathcal{D}(\Delta) = \mathcal{R}(T) \subset H_0^1(\Omega)$ described above.*

For a further description of $\mathcal{D}(\Delta)$, note that

$$(2.3) \quad \mathcal{D}(\Delta) = \{u \in H_0^1(\Omega) : \Delta u \in L^2(\Omega)\}.$$

If $\partial\Omega$ is smooth, we can apply the regularity theory of Chap. 5 to obtain

$$(2.4) \quad \mathcal{D}(\Delta) = H_0^1(\Omega) \cap H^2(\Omega).$$

Instead of relying on Proposition 8.2, we could use the Friedrichs construction, given in Proposition 8.7 of Appendix A. This construction can be applied more generally. Let Ω be any Riemannian manifold, with Laplace operator Δ . We can define $H_0^1(\Omega)$ to be the closure of $C_0^\infty(\Omega)$ in the space $\{u \in L^2(\Omega) : du \in L^2(\Omega, \Lambda^1)\}$. The inner product on $H_0^1(\Omega)$ is

$$(2.5) \quad (u, v)_1 = (u, v)_{L^2} + (du, dv)_{L^2}.$$

We have a natural inclusion $H_0^1(\Omega) \hookrightarrow L^2(\Omega)$, and the Friedrichs method gives a self-adjoint operator A on $L^2(\Omega)$ such that

$$(2.6) \quad (Au, v)_{L^2} = (u, v)_1, \quad \text{for } u \in \mathcal{D}(A), \quad v \in H_0^1(\Omega),$$

with

$$(2.7) \quad \mathcal{D}(A) = \{u \in H_0^1(\Omega) : v \mapsto (u, v)_1 \text{ extends from } H_0^1(\Omega) \rightarrow \mathbb{C} \text{ to a continuous linear functional } L^2(\Omega) \rightarrow \mathbb{C}\},$$

that is,

$$(2.8) \quad \mathcal{D}(A) = \{u \in H_0^1(\Omega) : \exists f \in L^2(\Omega) \text{ such that } (u, v)_1 = (f, v)_{L^2}, \forall v \in H_0^1(\Omega)\}.$$

Integrating (2.5) by parts for $v \in C_0^\infty(\Omega)$, we see that $A = I - \Delta$ on $\mathcal{D}(A)$, so we have a self-adjoint extension of Δ in this general setting, with domain again described by (2.3).

The process above gives one self-adjoint extension of Δ , initially defined on $C_0^\infty(\Omega)$. It is not always the only self-adjoint extension. For example, suppose $\overline{\Omega}$ is compact with smooth boundary; consider $H^1(\Omega)$, with inner product (2.5), and apply the Friedrichs extension procedure. Again we have a self-adjoint operator A , extending $I - \Delta$, with (2.8) replaced by

$$(2.9) \quad \mathcal{D}(A) = \{u \in H^1(\Omega) : \exists f \in L^2(\Omega) \text{ such that } (u, v)_1 = (f, v)_{L^2}, \forall v \in H^1(\Omega)\}.$$

In this case, Proposition 7.2 of Chap. 5 yields the following

Proposition 2.2. *If $\overline{\Omega}$ is a smooth, compact manifold with boundary and Δ the self-adjoint extension just described, then*

$$(2.10) \quad \mathcal{D}(\Delta) = \{u \in H^2(\Omega) : \partial_\nu u = 0 \text{ on } \partial\Omega\}.$$

In case (2.10), we say $\mathcal{D}(\Delta)$ is given by the Neumann boundary condition, while in case (2.4) we say $\mathcal{D}(\Delta)$ is given by the Dirichlet boundary condition.

In both cases covered by Propositions 2.1 and 2.2, $(-\Delta)^{1/2}$ is defined as a self-adjoint operator. We can specify its domain using Proposition 1.10, obtaining the next result:

Proposition 2.3. *In case (2.3), $\mathcal{D}((-\Delta)^{1/2}) = H_0^1(\Omega)$; in case (2.10), $\mathcal{D}((-\Delta)^{1/2}) = H^1(\Omega)$.*

Though Δ on $C_0^\infty(\Omega)$ has several self-adjoint extensions when Ω has a boundary, it has only one when Ω is a complete Riemannian manifold. This is a classical

result, due to Roelcke; we present an elegant proof due to Chernoff [Chn]. When an unbounded operator A_0 on a Hilbert space H , with domain \mathcal{D}_0 , has exactly one self-adjoint extension, namely the closure of A_0 , we say A_0 is *essentially self-adjoint* on \mathcal{D}_0 .

Proposition 2.4. *If Ω is a complete Riemannian manifold, then Δ is essentially self-adjoint on $C_0^\infty(\Omega)$. Thus the self-adjoint extension with domain given by (2.3) is the closure of Δ on $C_0^\infty(\Omega)$.*

Proof. We will obtain this as a consequence of Proposition 9.6 of Appendix A, which states the following. Let $U(t) = e^{itA}$ be a unitary group on a Hilbert space H which leaves invariant a dense linear space \mathcal{D} ; $U(t)\mathcal{D} \subset \mathcal{D}$. If A is an extension of A_0 and $A_0 : \mathcal{D} \rightarrow \mathcal{D}$, then A_0 and all its powers are essentially self-adjoint on \mathcal{D} .

In this case, $U(t)$ will be the solution operator for a wave equation, and we will exploit finite propagation speed. Set

$$(2.11) \quad iA_0 = \begin{pmatrix} 0 & I \\ \Delta - I & 0 \end{pmatrix}, \quad \mathcal{D}(A_0) = C_0^\infty(\Omega) \oplus C_0^\infty(\Omega).$$

The group $U(t)$ will be the solution operator for the wave equation

$$(2.12) \quad U(t) \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} u(t) \\ u_t(t) \end{pmatrix},$$

where $u(t, x)$ is determined by

$$\frac{\partial^2 u}{\partial t^2} - (\Delta - 1)u = 0; \quad u(0, x) = f, \quad u_t(0, x) = g$$

It was shown in §2 of Chap. 6 that $U(t)$ is a unitary group on $H = H_0^1(\Omega) \oplus L^2(\Omega)$; its generator is an extension of (2.11), and finite propagation speed implies that $U(t)$ preserves $C_0^\infty(\Omega) \oplus C_0^\infty(\Omega)$ for all t , provided Ω is complete. Thus each A_0^k is essentially self-adjoint on this space. Since

$$(2.13) \quad -A_0^2 = \begin{pmatrix} \Delta - I & 0 \\ 0 & \Delta - I \end{pmatrix},$$

we have the proof of Proposition 2.3. Considering A_0^{2k} , we deduce furthermore that each power Δ^k is essentially self-adjoint on $C_0^\infty(\Omega)$, when Ω is complete.

Though Δ is not essentially self-adjoint on $C_0^\infty(\Omega)$ when $\overline{\Omega}$ is compact, we do have such results as the following:

Proposition 2.5. *If $\overline{\Omega}$ is a smooth, compact manifold with boundary, then Δ is essentially self-adjoint on*

$$(2.14) \quad \{u \in C^\infty(\overline{\Omega}) : u = 0 \text{ on } \partial\Omega\},$$

its closure having domain described by (2.3). Also, Δ is essentially self-adjoint on

$$(2.15) \quad \{u \in C^\infty(\overline{\Omega}) : \partial_\nu u = 0 \text{ on } \partial\Omega\},$$

its closure having domain described by (2.10).

Proof. It suffices to note the simple facts that the closure of (2.14) in $H^2(\Omega)$ is (2.3) and the closure of (2.15) in $H^2(\Omega)$ is (2.10).

We note that when $\overline{\Omega}$ is a smooth, compact Riemannian manifold with boundary, and $\mathcal{D}(\Delta)$ is given by the Dirichlet boundary condition, then

$$(2.16) \quad \bigcap_{j=1}^{\infty} \mathcal{D}(\Delta^j) = \{u \in C^\infty(\overline{\Omega}) : \Delta^k u = 0 \text{ on } \partial\Omega, k = 0, 1, 2, \dots\},$$

and when $\mathcal{D}(\Delta)$ is given by the Neumann boundary condition, then

$$(2.17) \quad \bigcap_{j=1}^{\infty} \mathcal{D}(\Delta^j) = \{u \in C^\infty(\overline{\Omega}) : \partial_\nu(\Delta^k u) = 0 \text{ on } \partial\Omega, k \geq 0\}.$$

We now derive a result that to some degree amalgamates Propositions 2.4 and 2.5. Let $\overline{\Omega}$ be a smooth Riemannian manifold with boundary, and set

$$(2.18) \quad C_c^\infty(\overline{\Omega}) = \{u \in C^\infty(\overline{\Omega}) : \text{supp } u \text{ is compact in } \overline{\Omega}\};$$

we do not require elements of this space to vanish on $\partial\Omega$. We say that $\overline{\Omega}$ is complete if it is complete as a metric space.

Proposition 2.6. *If $\overline{\Omega}$ is a smooth Riemannian manifold with boundary which is complete, then Δ is essentially self-adjoint on*

$$(2.19) \quad \{u \in C_c^\infty(\overline{\Omega}) : u = 0 \text{ on } \partial\Omega\}.$$

In this case, the closure has domain given by (2.3).

Proof. Consider the following linear subspace of (2.19):

$$(2.20) \quad \mathcal{D}_0 = \{u \in C_c^\infty(\overline{\Omega}) : \Delta^j u = 0 \text{ on } \partial\Omega \text{ for } j = 0, 1, 2, \dots\}.$$

Let $U(t)$ be the unitary group on $H_0^1(\Omega) \oplus L^2(\Omega)$ defined as in (2.12), with u also satisfying the Dirichlet boundary condition, $u(t, x) = 0$ for $x \in \partial\Omega$. Then, by finite propagation speed, $U(t)$ preserves $\mathcal{D}_0 \oplus \mathcal{D}_0$, provided $\overline{\Omega}$ is complete, so as in the proof of Proposition 2.4, we deduce that Δ is essentially self-adjoint on \mathcal{D}_0 ; a fortiori it is essentially self-adjoint on the space (2.19).

By similar reasoning, we can show that if $\overline{\Omega}$ is complete, then Δ is essentially self-adjoint on

$$(2.21) \quad \{u \in C_c^\infty(\overline{\Omega}) : \partial_\nu u = 0 \text{ on } \partial\Omega\}.$$

The results of this section so far have involved only the Laplace operator Δ . It is also of interest to look at Schrödinger operators, of the form $-\Delta + V$, where the “potential” $V(x)$ is a real-valued function. In this section we will restrict attention to the case $V \in C^\infty(\Omega)$ and we will also suppose that V is bounded from below. By adding a constant to $-\Delta + V$, we may as well suppose

$$(2.22) \quad V(x) \geq 1 \text{ on } \Omega.$$

We can define a Hilbert space $H_{V0}^1(\Omega)$ to be the closure of $C_0^\infty(\Omega)$ in the space

$$(2.23) \quad H_V^1(\Omega) = \{u \in L^2(\Omega) : du \in L^2(\Omega, \Lambda^1), V^{1/2}u \in L^2(\Omega)\},$$

with inner product

$$(2.24) \quad (u, v)_{1,V} = (du, dv)_{L^2} + (Vu, v)_{L^2}.$$

Then there is a natural injection $H_{V0}^1(\Omega) \hookrightarrow L^2(\Omega)$, and the Friedrichs extension method provides a self-adjoint operator A . Integration by parts in (2.24), with $v \in C_0^\infty(\Omega)$, shows that such A is an extension of $-\Delta + V$. For this self-adjoint extension, we have

$$(2.25) \quad \mathcal{D}(A^{1/2}) = H_{V0}^1(\Omega).$$

In case $\overline{\Omega}$ is a smooth, compact Riemannian manifold with boundary and $V \in C^\infty(\overline{\Omega})$, one clearly has $H_{V0}^1(\Omega) = H_0^1(\Omega)$. In such a case, we have an immediate extension of Proposition 2.1, including the characterization (2.4) of $\mathcal{D}(-\Delta + V)$. One can also easily extend Proposition 2.2 to $-\Delta + V$ in this case. It is of substantial interest that Proposition 2.4 also extends, as follows:

Proposition 2.7. *If Ω is a complete Riemannian manifold and the function $V \in C^\infty(\Omega)$ satisfies $V \geq 1$, then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\Omega)$.*

Proof. We can modify the proof of Proposition 2.4; replace $\Delta - 1$ by $\Delta - V$ in (2.11) and (2.12). Then $U(t)$ gives a unitary group on $H_{V0}^1(\Omega) \oplus L^2(\Omega)$, and the finite propagation speed argument given there goes through. As before, all powers of $-\Delta + V$ are essentially self-adjoint on $C_0^\infty(\Omega)$.

Some important classes of potentials V have singularities and are not bounded below. In §7 we return to this, in a study of the quantum mechanical Coulomb problem.

We record here an important compactness property when $V \in C^\infty(\Omega)$ tends to $+\infty$ at infinity in Ω

Proposition 2.8. *If the Friedrichs extension method described above is used to construct the self-adjoint operator $-\Delta + V$ for smooth $V \geq 1$, as above, and if $V \rightarrow +\infty$ at infinity (i.e., for each $N < \infty$, $\Omega_N = \{x \in \Omega : V(x) \leq N\}$ is compact), then $-\Delta + V$ has compact resolvent.*

Proof. Given (2.25), it suffices to prove that the injection $H_{V_0}^1(\Omega) \rightarrow L^2(\Omega)$ is compact, under the current hypotheses on V . Indeed, if $\{u_n\}$ is bounded in $H_{V_0}^1(\Omega)$, with inner product (2.24), then $\{du_n\}$ and $\{V^{1/2}u_n\}$ are bounded in $L^2(\Omega)$. By Rellich's theorem and a diagonal argument, one has a subsequence $\{u_{n_k}\}$ whose restriction to each Ω_N converges in $L^2(\Omega_N)$ -norm. The boundedness of $\{V^{1/2}u_n\}$ in $L^2(\Omega)$ then gives convergence of this subsequence in $L^2(\Omega)$ -norm, proving the proposition.

The following result extends Proposition 2.4 of Chap. 5

Proposition 2.9. *Assume that Ω is connected and that either Ω is compact or $V \rightarrow +\infty$ at infinity. Denote by λ_0 the first eigenvalue of $-\Delta + V$. Then a λ_0 -eigenfunction of $-\Delta + V$ is nowhere vanishing on Ω . Consequently, the λ_0 -eigenspace is one-dimensional.*

Proof. Let u be a λ_0 -eigenfunction of $-\Delta + V$. As in the proof of Proposition 2.4 of Chap. 5, we can write $u = u^+ + u^-$, where $u^+(x) = u(x)$ for $u(x) > 0$ and $u^-(x) = u(x)$ for $u(x) \leq 0$, and the variational characterization of the λ_0 -eigenspace implies that u^\pm are eigenfunctions (if nonzero). Hence it suffices to prove that if u is a λ_0 -eigenfunction and $u(x) \geq 0$ on Ω , then $u(x) > 0$ on Ω . To this end, write

$$u(x) = e^{t(\Delta - V + \lambda_0)} u(x) = \int_{\Omega} p_t(x, y) u(y) dV(y)$$

We see that this forces $p_t(x, y) = 0$ for all $t > 0$, when

$$x \in \Sigma = \{x : u(x) = 0\}, \quad y \in \overline{\mathcal{O}}, \quad \mathcal{O} = \{x : u(x) > 0\},$$

since $p_t(x, y)$ is smooth and ≥ 0 . The strong maximum principle (see Exercise 3 in §1 of Chap. 6) forces $\Sigma = \emptyset$.

Exercises

1. Let $H_V^1(\Omega)$ be the space (2.23). If $V \geq 1$ belongs to $C^\infty(\Omega)$, show that the Friedrichs extension also defines a self-adjoint operator A_1 , equal to $-\Delta + V$ on $C_0^\infty(\Omega)$, such that $\mathcal{D}(A_1^{1/2}) = H_V^1(\Omega)$. If Ω is complete, show that this operator coincides with the extension A defined in (2.25). Conclude that, in this case, $H_V^1(\Omega) = H_{V_0}^1(\Omega)$.

2. Let Ω be complete, $V \geq 1$ smooth. Show that if A is the self-adjoint extension of $-\Delta + V$ described in Proposition 2.7, then

$$(2.26) \quad \mathcal{D}(A) = \{u \in L^2(\Omega) : -\Delta u + Vu \in L^2(\Omega)\},$$

where a priori we regard $-\Delta u + Vu$ as an element of $\mathcal{D}'(\Omega)$.

3. Define $T : L^2(\Omega) \rightarrow L^2(\Omega, \Lambda^1) \oplus L^2(\Omega)$ by $\mathcal{D}(T) = H_{V0}^1(\Omega)$, $Tu = (du, V^{1/2}u)$. Show that

$$(2.27) \quad \mathcal{D}(T^*) = \{(v_1, v_2) \in L^2(\Omega, \Lambda^1) \oplus L^2(\Omega) : \delta v_1 \in L^2(\Omega), V^{1/2}v_2 \in L^2(\Omega)\}.$$

Show that T^*T is equal to the self-adjoint extension A of $-\Delta + V$ defined by the Friedrichs extension, as in (2.25).

4. If Ω is complete, show that the self-adjoint extension A of $-\Delta + V$ in Proposition 2.7 satisfies

$$(2.28) \quad \mathcal{D}(A) = \{u \in L^2(\Omega) : \Delta u \in L^2(\Omega), Vu \in L^2(\Omega)\}.$$

(Hint: Denote the right side by \mathcal{W} . Use Exercise 3 and $A = T^*T$ to show that $\mathcal{D}(A) \subset \mathcal{W}$. Use Exercise 2 to show that $\mathcal{W} \subset \mathcal{D}(A)$.)

5. Let $D = -i d/dx$ on $C^\infty(\mathbb{R})$, and let $B(x) \in C^\infty(\mathbb{R})$ be real-valued. Define the unbounded operator L on $L^2(\mathbb{R})$ by

$$(2.29) \quad \mathcal{D}(L) = \{u \in L^2(\mathbb{R}) : Du \in L^2(\mathbb{R}), Bu \in L^2(\mathbb{R})\}, \quad Lu = Du + iB(x)u.$$

Show that $L^* = D - iB$, with

$$\mathcal{D}(L^*) = \{u \in L^2(\mathbb{R}) : Du - iBu \in L^2(\mathbb{R})\}$$

Deduce that $A_0 = L^*L$ is given by $A_0u = D^2u + B^2u + B'(x)u$ on

$$\mathcal{D}(A_0) = \{u \in L^2(\mathbb{R}) : Du \in L^2(\mathbb{R}), Bu \in L^2(\mathbb{R}), D^2u + B^2u + B'(x)u \in L^2(\mathbb{R})\}$$

6. Suppose that $|B'(x)| \leq \vartheta B(x)^2 + C$, for some $\vartheta < 1$, $C < \infty$. Show that

$$\mathcal{D}(A_0) = \{u \in L^2(\mathbb{R}) : D^2u + (B^2 + B')u \in L^2(\mathbb{R})\}$$

(Hint: Apply Exercise 2 to $D^2 + (B^2 + B') = A$, and show that $\mathcal{D}(A^{1/2})$ is given by $\mathcal{D}(L)$, defined in (2.29).)

7. In the setting of Exercise 6, show that the operator L of Exercise 5 is closed.

(Hint: $L^*\bar{L} = A$ is a self-adjoint extension of $D^2 + (B^2 + B')$. Show that $\mathcal{D}(A_1^{1/2}) = \mathcal{D}(L)$ and also $= \mathcal{D}(\bar{L})$.) Also show that $\mathcal{D}(L^*) = \mathcal{D}(L)$ in this case.

3. Heat asymptotics and eigenvalue asymptotics

In this section we will study the asymptotic behavior of the eigenvalues of the Laplace operator on a compact Riemannian manifold, with or without boundary.

We begin with the boundaryless case. Let M be a compact Riemannian manifold without boundary, of dimension n . In §13 of Chap. 7 we have constructed a parametrix for the solution operator $e^{t\Delta}$ of the heat equation

$$(3.1) \quad \left(\frac{\partial}{\partial t} - \Delta\right)u = 0 \text{ on } \mathbb{R}^+ \times M, \quad u(0, x) = f(x)$$

and deduced that

$$(3.2) \quad \text{Tr } e^{t\Delta} \sim t^{-n/2} (a_0 + a_1 t + a_2 t^2 + \cdots), \quad t \searrow 0,$$

for certain constants a_j . In particular,

$$(3.3) \quad a_0 = (4\pi)^{-n/2} \text{vol } M.$$

This is related to the behavior of the eigenvalues of Δ as follows. Let the eigenvalues of $-\Delta$ be $0 = \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \cdots \nearrow \infty$. Then (3.2) is equivalent to

$$(3.4) \quad \sum_{j=0}^{\infty} e^{-t\lambda_j} \sim t^{-n/2} (a_0 + a_1 t + a_2 t^2 + \cdots), \quad t \searrow 0.$$

We will relate this to the counting function

$$(3.5) \quad N(\lambda) \sim \#\{\lambda_j : \lambda_j \leq \lambda\},$$

establishing the following:

Theorem 3.1. *The eigenvalues $\{\lambda_j\}$ of $-\Delta$ on the compact Riemannian manifold M have the behavior*

$$(3.6) \quad N(\lambda) \sim C(M) \lambda^{n/2}, \quad \lambda \rightarrow +\infty,$$

with

$$(3.7) \quad C(M) = \frac{a_0}{\Gamma(\frac{n}{2} + 1)} = \frac{\text{vol } M}{\Gamma(\frac{n}{2} + 1)(4\pi)^{n/2}}.$$

That (3.6) follows from (3.4) is a special case of a result known as *Karamata's Tauberian theorem*. The following neat proof follows one in [Si3]. Let μ be a positive (locally finite) Borel measure on $[0, \infty)$; in the example above, $\mu([0, \lambda]) = N(\lambda)$.

Proposition 3.2. *If μ is a positive measure on $[0, \infty)$, $\alpha \in (0, \infty)$, then*

$$(3.8) \quad \int_0^\infty e^{-t\lambda} d\mu(\lambda) \sim at^{-\alpha}, \quad t \searrow 0,$$

implies

$$(3.9) \quad \int_0^x d\mu(\lambda) \sim bx^\alpha, \quad x \nearrow \infty,$$

with

$$(3.10) \quad b = \frac{a}{\Gamma(\alpha + 1)}.$$

Proof. Let $d\mu_t$ be the measure given by $\mu_t(A) = t^\alpha \mu(t^{-1}A)$, and let $d\nu(\lambda) = \alpha \lambda^{\alpha-1} d\lambda$; then $\nu_t = \nu$. The hypothesis (3.8) becomes

$$(3.11) \quad \lim_{t \rightarrow 0} \int e^{-\lambda} d\mu_t(\lambda) = b \int e^{-\lambda} d\nu(\lambda),$$

with b given by (3.10), and the desired conclusion becomes

$$(3.12) \quad \lim_{t \rightarrow 0} \int \chi(\lambda) d\mu_t(\lambda) = b \int \chi(\lambda) d\nu(\lambda)$$

when χ is the characteristic function of $[0, 1]$. It would suffice to show that (3.12) holds for all continuous $\chi(\lambda)$ with compact support in $[0, \infty)$.

From (3.11) we deduce that the measures $e^{-\lambda} d\mu_t$ are uniformly bounded, for $t \in (0, 1]$. Thus (3.12) follows if we can establish

$$(3.13) \quad \lim_{t \rightarrow 0} \int g(\lambda) e^{-\lambda} d\mu_t(\lambda) = b \int g(\lambda) e^{-\lambda} d\nu(\lambda),$$

for g in a dense subspace of $C_0(\mathbb{R}^+)$, the space of continuous functions on $[0, \infty)$ that vanish at infinity. Indeed, the hypothesis implies that (3.13) holds for all g in \mathfrak{A} , the space of finite, linear combinations of functions of $\lambda \in [0, \infty)$ of the form $\varphi_s(\lambda) = e^{-s\lambda}$, $s \in (0, \infty)$, as can be seen by dilating the variables in (3.11). By the Stone-Weierstrass theorem, \mathfrak{A} is dense in $C_o(\mathbb{R}^+)$, so the proof is complete.

We next want to establish similar results on $N(\lambda)$ for the Laplace operator Δ on a compact manifold $\overline{\Omega}$ with boundary, with Dirichlet boundary condition. At the end of §13 in Chap. 7 we sketched a construction of a parametrix for $e^{t\Delta}$ in this case which, when carried out, would yield an expansion

$$(3.14) \quad \text{Tr } e^{t\Delta} \sim t^{-n/2} (a_0 + a_{1/2} t^{1/2} + a_1 t + \cdots), \quad t \searrow 0,$$

extending (3.2). However, we will be able to verify the hypothesis of Proposition 3.2 with less effort than it would take to carry out the details of this construction, and for a much larger class of domains.

For simplicity, we will restrict attention to bounded domains in \mathbb{R}^n and to the flat Laplacian, though more general cases can be handled similarly. Now, let Ω be an arbitrary bounded, open subset of \mathbb{R}^n , with closure $\overline{\Omega}$. The Laplace operator on Ω , with Dirichlet boundary condition, was studied in §5 of Chap. 5

Lemma 3.3. *For any bounded, open $\Omega \subset \mathbb{R}^n$, Δ with Dirichlet boundary condition, $e^{t\Delta}$ is trace class for all $t > 0$.*

Proof. Let $\overline{\Omega} \subset B$, a large open ball. Then the variational characterization of eigenvalues shows that the eigenvalues $\lambda_j(\Omega)$ of $-\Delta$ on Ω and $\lambda_j(B)$ of $L = -\Delta$ on B , both arranged in increasing order, have the relation

$$(3.15) \quad \lambda_j(\Omega) \geq \lambda_j(B).$$

But we know that e^{-tL} has integral kernel in $C^\infty(\overline{B} \times \overline{B})$ for each $t > 0$, hence is trace class. Since $e^{-t\lambda_j(\Omega)} \leq e^{-t\lambda_j(B)}$, this implies that the positive self-adjoint operator $e^{t\Delta}$ is also trace class.

Limiting arguments, which we leave to the reader, allow one to show that, even in this generality, if $H(t, x, y) \in C^\infty(\Omega \times \Omega)$ is, for fixed $t > 0$, the integral kernel of $e^{t\Delta}$ on $L^2(\Omega)$, then

$$(3.16) \quad \text{Tr } e^{t\Delta} = \int_{\Omega} H(t, x, x) \, dx.$$

See Exercises 1–5 at the end of this section.

Proposition 3.4. *If Ω is a bounded, open subset of \mathbb{R}^n and Δ has the Dirichlet boundary condition, then*

$$(3.17) \quad \text{Tr } e^{t\Delta} \sim (4\pi t)^{-n/2} \text{vol } \Omega, \quad t \searrow 0.$$

Proof. We will compare $H(t, x, y)$ with $H_0(t, x, y) = (4\pi t)^{-n/2} e^{|x-y|^2/4t}$, the free-space heat kernel. Let $E(t, x, y) = H_0(t, x, y) - H(t, x, y)$. Then, for fixed $y \in \Omega$,

$$(3.18) \quad \frac{\partial E}{\partial t} - \Delta_x E = 0 \text{ on } \mathbb{R}^+ \times \Omega, \quad E(0, x, y) = 0,$$

and

$$(3.19) \quad E(t, x, y) = H_0(t, x, y), \quad \text{for } x \in \partial\Omega.$$

To make simple sense out of (3.19), one might assume that every point of $\partial\Omega$ is a regular boundary point, though a further limiting argument can be made to lift such a restriction. The maximum principle for solutions to the heat equation implies

$$(3.20) \quad 0 \leq E(t, x, y) \leq \sup_{0 \leq s \leq t, z \in \Omega} H_0(s, z, y) \leq \sup_{0 \leq s \leq t} (4\pi s)^{-n/2} e^{-\delta(y)^2/4s},$$

where $\delta(y) = \text{dist}(y, \partial\Omega)$. Now the function

$$\psi_\delta(s) = (4\pi s)^{-n/2} e^{-\delta^2/4s}$$

on $(0, \infty)$ vanishes at 0 and ∞ and has a unique maximum at $s = \delta^2/2n$; we have $\psi_\delta(\delta^2/2n) = C_n \delta^{-n}$. Thus

$$(3.21) \quad 0 \leq E(t, x, y) \leq \max\left((4\pi t)^{-n/2} e^{-\delta(y)^2/4t}, C_n \delta(y)^{-n}\right).$$

Of course, $E(t, x, y) \leq H_0(t, x, y)$ also.

Now, let $\overline{\mathcal{O}} \subset \subset \Omega$ be such that $\text{vol}(\Omega \setminus \mathcal{O}) < \varepsilon$. For t small enough, namely for $t \leq \delta_1^2/2n$ where $\delta_1 = \text{dist}(\overline{\mathcal{O}}, \partial\Omega)$, we have

$$(3.22) \quad 0 \leq E(t, x, x) \leq (4\pi t)^{-n/2} e^{-\delta(x)^2/4t}, \quad x \in \mathcal{O},$$

while of course $0 \leq E(t, x, x) \leq (4\pi t)^{-n/2}$, for $x \in \Omega \setminus \mathcal{O}$. Therefore,

$$(3.23) \quad \limsup_{t \rightarrow 0} (4\pi t)^{n/2} \int_{\Omega} E(t, x, x) dx \leq \varepsilon,$$

so

$$(3.24) \quad \begin{aligned} \text{vol } \Omega - \varepsilon &\leq \liminf_{t \rightarrow 0} (4\pi t)^{n/2} \int_{\Omega} H(t, x, x) dx \\ &\leq \limsup_{t \rightarrow 0} (4\pi t)^{n/2} \int_{\Omega} H(t, x, x) dx \leq \text{vol } \Omega. \end{aligned}$$

As ε can be taken arbitrarily small, we have a proof of (3.17).

Corollary 3.5. *If Ω is a bounded, open subset of \mathbb{R}^n , $N(\lambda)$ the counting function of the eigenvalues of $-\Delta$, with Dirichlet boundary condition, then (3.6) holds.*

Note that if \mathcal{O}_ε is the set of points in Ω of distance $\geq \varepsilon$ from $\partial\Omega$ and we define $v(\varepsilon) = \text{vol}(\Omega \setminus \mathcal{O}_\varepsilon)$, then the estimate (3.24) can be given the more precise reformulation

$$(3.25) \quad 0 \leq \text{vol } \Omega - (4\pi t)^{n/2} \text{Tr } e^{t\Delta} \leq \omega(\sqrt{2nt}),$$

where

$$(3.26) \quad \omega(\varepsilon) = v(\varepsilon) + \int_{\varepsilon}^{\infty} e^{-ns^2/2\varepsilon^2} dv(s).$$

The fact that such a crude argument works, and works so generally, is a special property of the Dirichlet problem. If one uses the Neumann boundary condition, then for bounded $\Omega \subset \mathbb{R}^n$ with nasty boundary, Δ need not even have compact resolvent. However, Theorem 3.1 does extend to the Neumann boundary condition provided $\partial\Omega$ is smooth. One can do this via the sort of parametrix for boundary problems sketched in §13 of Chap. 7.

We now look at the heat kernel $H(t, x, y)$ on the *complement* of a smooth, bounded region $K \subset \mathbb{R}^n$. We impose the Dirichlet boundary condition on ∂K . As before, $0 \leq H(t, x, y) \leq H_0(t, x, y)$, where $H_0(t, x, y)$ is the free-space heat kernel. We can extend $H(t, x, y)$ to be Lipschitz continuous on $(0, \infty) \times \mathbb{R}^n \times \mathbb{R}^n$ by setting $H(t, x, y) = 0$ when either $x \in K$ or $y \in K$. We now estimate $E(t, x, y) = H_0(t, x, y) - H(t, x, y)$. Suppose K is contained in the open ball of radius R centered at the origin.

Lemma 3.6. *For $|x - y| \leq |y| - R$, we have*

$$(3.27) \quad E(t, x, y) \leq C t^{-1/2} e^{-(|y|-R)^2/4t}.$$

Proof. With $y \in \Omega = \mathbb{R}^n \setminus K$, write

$$(3.28) \quad H(t, x, y) = (4\pi t)^{-1/2} \int_{-\infty}^{\infty} e^{-s^2/4t} \cos s\Lambda \, ds,$$

where $\Lambda = \sqrt{-\Delta}$ and Δ is the Laplace operator on Ω , with the Dirichlet boundary condition. We have a similar formula for $H_0(t, x, y)$, using instead $\Lambda_0 = \sqrt{-\Delta_0}$, with Δ_0 the free-space Laplacian. Now, by finite propagation speed,

$$\cos s\Lambda \, \delta_y(x) = \cos s\Lambda_0 \, \delta_y(x),$$

provided

$$|s| \leq d = \text{dist}(y, \partial K), \text{ and } |x - y| \leq d$$

Thus, as long as $|x - y| \leq d$, we have

$$(3.29) \quad E(t, x, y) = (4\pi t)^{-1/2} \int_{|s| \geq d} e^{-s^2/4t} [\cos s\Lambda_0 \, \delta_y(x) - \cos s\Lambda \, \delta_y(x)] \, ds.$$

Then the estimate (3.27) follows easily, along the same lines as estimates on heat kernels discussed in Chap. 6, §2.

When we combine (3.27) with the obvious inequality

$$(3.30) \quad 0 \leq E(t, x, y) \leq H_0(t, x, y) = (4\pi t)^{-n/2} e^{-|x-y|^2/4t},$$

we see that, for each $t > 0$, $E(t, x, y)$ is rapidly decreasing as $|x| + |y| \rightarrow \infty$. Using this and appropriate estimates on derivatives, we can show that $E(t, x, y)$ is the integral kernel of a trace class operator on $L^2(\mathbb{R}^n)$. We can write

$$(3.31) \quad \text{Tr} (e^{t\Delta_0} - e^{t\Delta} P) = \int_{\mathbb{R}^n} E(t, x, x) dx,$$

where P is the projection of $L^2(\mathbb{R}^n)$ onto $L^2(\Omega)$ defined by restriction to Ω . Now, as $t \searrow 0$, $(4\pi t)^{n/2} E(t, x, x)$ approaches 1 on K and 0 on $\mathbb{R}^n \setminus K$. Together with the estimates (3.27) and (3.30), this implies

$$(3.32) \quad (4\pi t)^{n/2} \int_{\mathbb{R}^n} E(t, x, x) dx \longrightarrow \text{vol } K,$$

as $t \searrow 0$. This establishes the following:

Proposition 3.7. *If K is a closed, bounded set in \mathbb{R}^n , Δ is the Laplacian on $L^2(\mathbb{R}^n \setminus K)$, with Dirichlet boundary condition, and Δ_0 is the Laplacian on $L^2(\mathbb{R}^n)$, then $e^{t\Delta_0} - e^{t\Delta} P$ is trace class for each $t > 0$ and*

$$(3.33) \quad \text{Tr} (e^{t\Delta_0} - e^{t\Delta} P) \sim (4\pi t)^{-n/2} \text{vol } K,$$

as $t \searrow 0$.

This result will be of use in the study of scattering by an obstacle K , in Chap. 9. It is also valid for the Neumann boundary condition if ∂K is smooth.

Exercises

In Exercises 1–4, let $\Omega \subset \mathbb{R}^n$ be a bounded, open set and let \mathcal{O}_j be open with smooth boundary such that

$$\mathcal{O}_1 \subset \subset \mathcal{O}_2 \subset \subset \cdots \subset \subset \mathcal{O}_j \subset \subset \cdots \nearrow \Omega.$$

Let L_j be $-\Delta$ on \mathcal{L}_j , with Dirichlet boundary condition; the corresponding operator on Ω is simply denoted $-\Delta$.

- Using material developed in §5 of Chap. 5, show that, for any $t > 0$, $f \in L^2(\Omega)$,

$$e^{-tL_j} P_j f \longrightarrow e^{t\Delta} f \text{ strongly in } L^2(\Omega),$$

as $j \rightarrow \infty$, where P_j is multiplication by the characteristic function of \mathcal{O}_j .

Don't peek at Lemma 3.4 in Chap. 11!

- If $\lambda_\nu(\mathcal{O}_j)$ are the eigenvalues of L_j , arranged in increasing order for each j , show that, for each ν ,

$$\lambda_\nu(\mathcal{O}_j) \searrow \lambda_\nu(\Omega), \text{ as } j \rightarrow \infty.$$

- Show that, for each $t > 0$,

$$\text{Tr } e^{-tL_j} \nearrow \text{Tr } e^{t\Delta}.$$

- Let $H_j(t, x, y)$ be the heat kernel on $\mathbb{R}^+ \times \overline{\mathcal{O}_j} \times \overline{\mathcal{O}_j}$. Extend H_j to $\mathbb{R}^+ \times \Omega \times \Omega$ so as to vanish if x or y belongs to $\Omega \setminus \mathcal{O}_j$. Show that, for each $x \in \Omega$, $y \in \Omega$, $t > 0$,

$$H_j(t, x, y) \nearrow H(t, x, y), \text{ as } j \rightarrow \infty.$$

Deduce that, for each $t > 0$,

$$\int_{\mathcal{O}_j} H_j(t, x, x) dx \nearrow \int_{\Omega} H(t, x, x) dx$$

5. Using Exercises 1–4, give a detailed proof of (3.16) for general bounded $\Omega \subset \mathbb{R}^n$.
6. Give an example of a bounded, open, connected set $\Omega \subset \mathbb{R}^2$ (with rough boundary) such that Δ , with Neumann boundary condition, does not have compact resolvent.

4. The Laplace operator on S^n

A key tool in the analysis of the Laplace operator Δ_S on S^n is the formula for the Laplace operator on \mathbb{R}^{n+1} in polar coordinates:

$$(4.1) \quad \Delta = \frac{\partial^2}{\partial r^2} + \frac{n}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \Delta_S.$$

In fact, this formula is simultaneously the main source of interest in Δ_S and the best source of information about it.

To begin, we consider the Dirichlet problem for the unit ball in Euclidean space, $B = \{x \in \mathbb{R}^{n+1} : |x| < 1\}$:

$$(4.2) \quad \Delta u = 0 \text{ in } B, \quad u = f \text{ on } S^n = \partial B,$$

given $f \in \mathcal{D}'(S^n)$. In Chap. 5 we obtained the Poisson integral formula for the solution:

$$(4.3) \quad u(x) = \frac{1 - |x|^2}{A_n} \int_{S^n} \frac{f(y)}{|x - y|^{n+1}} dS(y),$$

where A_n is the volume of S^n . Equivalently, if we set $x = r\omega$ with $r = |x|$, $\omega \in S^n$,

$$(4.4) \quad u(r\omega) = \frac{1 - r^2}{A_n} \int_{S^n} \frac{f(\omega')}{(1 - 2r\omega \cdot \omega' + r^2)^{(n+1)/2}} dS(\omega').$$

Now we can derive an alternative formula for the solution of (4.2) if we use (4.1) and regard $\Delta u = 0$ as an operator-valued ODE in r ; it is an Euler equation, with solution

$$(4.5) \quad u(r\omega) = r^{A-(n-1)/2} f(\omega), \quad r \leq 1,$$

where A is an operator on $\mathcal{D}'(S^n)$, defined by

$$(4.6) \quad A = \left(-\Delta_S + \frac{(n-1)^2}{4} \right)^{1/2}.$$

If we set $r = e^{-t}$ and compare (4.5) and (4.4), we obtain a formula for the semigroup e^{-tA} as follows. Let $\theta(\omega, \omega')$ denote the geodesic distance on S^n from ω to ω' , so $\cos \theta(\omega, \omega') = \omega \cdot \omega'$. We can rewrite (4.4) as

$$(4.7) \quad u(r\omega) = \frac{2}{A_n} \sinh(\log r^{-1}) r^{-(n-1)/2} \cdot \int_{S^n} \frac{f(\omega')}{[2 \cosh(\log r^{-1}) - 2 \cos \theta(\omega, \omega')]^{(n+1)/2}} dS(\omega').$$

In other words, by (4.5),

$$(4.8) \quad e^{-tA} f(\omega) = \frac{2}{A_n} \sinh t \int_{S^n} \frac{f(\omega')}{(2 \cosh t - 2 \cos \theta(\omega, \omega'))^{(n+1)/2}} dS(\omega').$$

Identifying an operator on $\mathcal{D}'(S^n)$ with its Schwartz kernel in $\mathcal{D}'(S^n \times S^n)$, we write

$$(4.9) \quad e^{-tA} = \frac{2}{A_n} \frac{\sinh t}{(2 \cosh t - 2 \cos \theta)^{(n+1)/2}}, \quad t > 0.$$

Note that the integration of (4.9) from t to ∞ produces the formula

$$(4.10) \quad A^{-1} e^{-tA} = 2C_n (2 \cosh t - 2 \cos \theta)^{-(n-1)/2}, \quad t > 0,$$

provided $n \geq 2$, where

$$C_n = \frac{1}{(n-1)A_n} = \frac{1}{4} \pi^{-(n+1)/2} \Gamma\left(\frac{n-1}{2}\right)$$

With the exact formula (4.9) for the semigroup e^{-tA} , we can proceed to give formulas for fundamental solutions to various important PDE, particularly

$$(4.11) \quad \frac{\partial^2 u}{\partial t^2} - Lu = 0 \quad (\text{wave equation})$$

and

$$(4.12) \quad \frac{\partial u}{\partial t} - Lu = 0 \quad (\text{heat equation}),$$

where

$$(4.13) \quad L = \Delta_S - \frac{(n-1)^2}{4} = -A^2.$$

If we prescribe Cauchy data $u(0) = f$, $u_t(0) = g$ for (4.11), the solution is

$$(4.14) \quad u(t) = (\cos tA) f + A^{-1} (\sin tA) g.$$

Assume $n \geq 2$. We obtain formulas for these terms by analytic continuation of the formulas (4.9) and (4.10) to $\operatorname{Re} t > 0$ and then passing to the limit $t \in i\mathbb{R}$. This is parallel to the derivation of the fundamental solution to the wave equation on Euclidean space in §5 of Chap. 3. We have

$$(4.15) \quad \begin{aligned} A^{-1} e^{(it-\varepsilon)A} &= -2C_n [2 \cosh(it - \varepsilon) - 2 \cos \theta]^{-(n-1)/2}, \\ e^{(it-\varepsilon)A} &= \frac{2}{A_n} \sinh(it - \varepsilon) [2 \cosh(it - \varepsilon) - 2 \cos \theta]^{-(n+1)/2}. \end{aligned}$$

Letting $\varepsilon \searrow 0$, we have

$$(4.16) \quad \begin{aligned} &A^{-1} \sin t A = \\ \lim_{\varepsilon \searrow 0} &-2C_n \operatorname{Im} (2 \cosh \varepsilon \cos t - 2i \sinh \varepsilon \sin t - 2 \cos \theta)^{-(n-1)/2} \end{aligned}$$

and

$$(4.17) \quad \begin{aligned} &\cos t A = \\ \lim_{\varepsilon \searrow 0} &\frac{-2}{A_n} \operatorname{Im}(\sin t) (2 \cosh \varepsilon \cos t - 2i \sinh \varepsilon \sin t - 2 \cos \theta)^{-(n+1)/2}. \end{aligned}$$

For example, on S^2 we have, for $0 \leq t \leq \pi$,

$$(4.18) \quad \begin{aligned} A^{-1} \sin t A &= -2C_2 (2 \cos \theta - 2 \cos t)^{-1/2}, & \theta < |t|, \\ &0, & \theta > |t|, \end{aligned}$$

with an analogous expression for general t , determined by the identity

$$(4.19) \quad A^{-1} \sin(t + 2\pi)A = -A^{-1} \sin t A \quad \text{on } \mathcal{D}'(S^{2k}),$$

plus the fact that $\sin t A$ is odd in t . The last line on the right in (4.18) reflects the well-known finite propagation speed for solutions to the hyperbolic equation (4.11).

To understand how the sign is determined in (4.19), note that, in (4.15), with $\varepsilon > 0$, for $t = 0$ we have a real kernel, produced by taking the $-(n-1)/2 = -k + 1/2$ power of a positive quantity. As t runs from 0 to 2π , the quantity $2 \cosh(it - \varepsilon) = 2 \cosh \varepsilon \cos t - 2i \sinh \varepsilon \sin t$ moves once clockwise around a circle of radius $2(\cosh^2 \varepsilon + \sinh^2 \varepsilon)^{1/2}$, centered at 0, so $2 \cosh \varepsilon \cos t - 2i \sinh \varepsilon \sin t - 2 \cos \theta$ describes a curve winding once clockwise about the origin in \mathbb{C} . Thus taking a half-integral power of this gives one the negative sign in (4.14).

On the other hand, when n is odd, the exponents on the right side of (4.15)–(4.17) are integers. Thus

$$(4.20) \quad A^{-1} \sin(t + 2\pi)A = A^{-1} \sin t A \quad \text{on } \mathcal{D}'(S^{2k+1}).$$

Also, in this case, the distributional kernel for $A^{-1} \sin t A$ must vanish for $|t| \neq \theta$. In other words, the kernel is supported on the shell $\theta = |t|$. This is the generalization to spheres of the strict Huygens principle.

In case $n = 2k + 1$ is odd, we obtain from (4.16) and (4.17) that

$$(4.21) \quad A^{-1} \sin t A f(x) = \frac{1}{(2k-1)!!} \left(\frac{1}{\sin s} \frac{\partial}{\partial s} \right)^{k-1} (\sin^{2k-1} s \bar{f}(x, s))_{s=t}$$

and

$$(4.22) \quad \cos t A f(x) = \frac{1}{(2k-1)!!} \sin s \left(\frac{1}{\sin s} \frac{\partial}{\partial s} \right)^k (\sin^{2k-1} s \bar{f}(x, s))_{s=t},$$

where, as in (5.66) of Chap. 3, $(2k-1)!! = 3 \cdot 5 \cdots (2k-1)$ and

$$(4.23) \quad \bar{f}(x, s) = \text{mean value of } f \text{ on } \Sigma_s(x) = \{y \in S^n : \theta(x, y) = |s|\}.$$

We can examine general functions of the operator A by the functional calculus

$$(4.24) \quad g(A) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \hat{g}(t) e^{itA} dt = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \hat{g}(t) \cos tA dt,$$

where the last identity holds provided g is an even function. We can rewrite this, using the fact that $\cos tA$ has period 2π in t on $\mathcal{D}'(S^n)$ for n odd, period 4π for n even. In concert with (4.22), we have the following formula for the Schwartz kernel of $g(A)$ on $\mathcal{D}'(S^{2k+1})$, for g even:

$$(4.25) \quad g(A) = (2\pi)^{-1/2} \left(-\frac{1}{2\pi} \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \right)^k \sum_{k=-\infty}^{\infty} \hat{g}(\theta + 2k\pi).$$

As an example, we compute the heat kernel on odd-dimensional spheres. Take $g(\lambda) = e^{-t\lambda^2}$. Then $\hat{g}(s) = (2t)^{-1/2} e^{-s^2/4t}$ and

$$(4.26) \quad (2\pi)^{-1/2} \sum_k \hat{g}(s + 2k\pi) = (4\pi t)^{-1/2} \sum_k e^{-(s+2k\pi)^2/4t} = \vartheta(s, t),$$

where $\vartheta(s, t)$ is a “theta function.” Thus the kernel of e^{-tA^2} on S^{2k+1} is given by

$$(4.27) \quad e^{-tA^2} = \left(-\frac{1}{2\pi} \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \right)^k \vartheta(\theta, t).$$

A similar analysis on S^{2k} gives an integral, with the theta function appearing in the integrand.

The operator A has a compact resolvent on $L^2(S^n)$, and hence a discrete set of eigenvalues, corresponding to an orthonormal basis of eigenfunctions. Indeed, the spectrum of A has the following description

Proposition 4.1. *The spectrum of the self-adjoint operator A on $L^2(S^n)$ is*

$$(4.28) \quad \text{spec } A = \left\{ \frac{1}{2}(n-1) + k : k = 0, 1, 2, \dots \right\}.$$

Proof. Since 0 is the smallest eigenvalue of $-\Delta_S$, the definition (4.6) shows that $(n-1)/2$ is the smallest eigenvalue of A . Also, (4.20) shows that all eigenvalues of A are integers if n is odd, while (4.19) implies that all eigenvalues of A are (nonintegral) half-integers if n is even. Thus $\text{spec } A$ is certainly contained in the right side of (4.28).

Another way to see this containment is to note that since the function $u(x)$ given by (4.5) must be smooth at $x = 0$, the exponent of r in that formula can take only integer values.

Let V_k denote the eigenspace of A with eigenvalue $v_k = (n-1)/2 + k$. We want to show that $V_k \neq 0$ for $k = 0, 1, 2, \dots$. Moreover, we want to identify V_k . Now if $f \in V_k$, it follows that $u(x) = u(r\omega) = r^{A-(n-1)/2} f(\omega) = r^k f(\omega)$ is a harmonic function defined on all of \mathbb{R}^{n+1} , which, being homogeneous and smooth at $x = 0$, must be a harmonic polynomial, homogeneous of degree k in x . If \mathcal{H}_k denotes the space of harmonic polynomials, homogeneous of degree k , restriction to $S^n \subset \mathbb{R}^{n+1}$ produces an isomorphism:

$$(4.29) \quad \rho : \mathcal{H}_k \xrightarrow{\approx} V_k.$$

To show that each $V_k \neq 0$, it suffices to show that each $\mathcal{H}_k \neq 0$.

Indeed, for $c = (c_1, \dots, c_{n+1}) \in \mathbb{C}^{n+1}$, consider

$$p_c(x) = (c_1 x_1 + \dots + c_{n+1} x_{n+1})^k.$$

A computation gives

$$\begin{aligned} \Delta p_c(x) &= k(k-1) \langle c, c \rangle (c_1 x_1 + \dots + c_k x_k)^{k-2}, \\ \langle c, c \rangle &= c_1^2 + \dots + c_k^2. \end{aligned}$$

Hence $\Delta p_c = 0$ whenever $\langle c, c \rangle = 0$, so the proposition is proved.

We now want to specify the orthogonal projections E_k of $L^2(S^n)$ on V_k . We can attack this via (4.10), which implies

$$(4.30) \quad \sum_{k=0}^{\infty} v_k^{-1} e^{-t v_k} E_k(x, y) = 2C_n (2 \cosh t - 2 \cos \theta)^{-(n-1)/2},$$

where $\theta = \theta(x, y)$ is the geodesic distance from x to y in S^n . If we set $r = e^{-t}$ and use $v_k = (n-1)/2 + k$, we get the generating function identity

$$(4.31) \quad \sum_{k=0}^{\infty} r^k v_k^{-1} E_k(x, y) = 2C_n(1 - 2r \cos \theta + r^2)^{-(n-1)/2} \\ = \sum_{k=0}^{\infty} r^k p_k(\cos \theta);$$

in particular,

$$(4.32) \quad E_k(x, y) = v_k p_k(\cos \theta).$$

These functions are polynomials in $\cos \theta$. To see this, set $t = \cos \theta$ and write

$$(4.33) \quad (1 - 2tr + r^2)^{-\alpha} = \sum_{k=0}^{\infty} C_k^\alpha(t) r^k,$$

thus defining coefficients $C_k^\alpha(t)$. To compute these, use

$$(1 - z)^{-\alpha} = \sum_{j=0}^{\infty} \binom{j + \alpha - 1}{j} z^j,$$

with $z = r(2t - r)$, to write the left side of (4.33) as

$$\sum_{j=0}^{\infty} \binom{\alpha}{j} r^j (2t - r)^j = \sum_{j=0}^{\infty} \sum_{\ell=0}^j \binom{j + \alpha - 1}{j} \binom{j}{\ell} (-1)^\ell r^{j+\ell} (2t)^{j-\ell} \\ = \sum_{k=0}^{\infty} \sum_{\ell=0}^{[k/2]} (-1)^\ell \binom{k - \ell + \alpha - 1}{k - \ell} \binom{k - \ell}{\ell} (2t)^{k-2\ell} r^k.$$

Hence

$$(4.34) \quad C_k^\alpha(t) = \sum_{\ell=0}^{[k/2]} (-1)^\ell \binom{k - \ell + \alpha - 1}{k - \ell} \binom{k - \ell}{\ell} (2t)^{k-2\ell}.$$

These are called *Gegenbauer polynomials*. Therefore, we have the following:

Proposition 4.2. *The orthogonal projection of $L^2(S^n)$ onto V_k has kernel*

$$(4.35) \quad E_k(x, y) = 2C_n v_k C_k^\alpha(\cos \theta), \quad \alpha = \frac{1}{2}(n-1),$$

with C_n as in (4.10).

In the special case $n = 2$, we have $C_2 = 1/4\pi$, and $v_k = k + 1/2$; hence

$$(4.36) \quad E_k(x, y) = \frac{2k+1}{4\pi} C_k^{1/2}(\cos \theta) = \frac{2k+1}{4\pi} P_k(\cos \theta),$$

where $C_k^{1/2}(t) = P_k(t)$ are the *Legendre polynomials*.

The trace of E_k is easily obtained by integrating (4.35) over the diagonal, to yield

$$(4.37) \quad \text{Tr } E_k = 2C_n A_n v_k C_k^{(n-1)/2}(1) = \frac{2v_k}{n-1} C_k^{(n-1)/2}(1).$$

Setting $t = 1$ in (4.33), so $(1 - 2r + r^2)^{-\alpha} = (1 - r)^{-2\alpha}$, we obtain

$$(4.38) \quad C_k^\alpha(1) = \binom{k+2\alpha-1}{k}, \quad \text{e.g., } P_k(1) = 1.$$

Thus we have the dimensions of the eigenspaces V_k :

Corollary 4.3. *The eigenspace V_k of $-\Delta_S$ on S^n , with eigenvalue*

$$\lambda_k = v_k^2 - \frac{1}{4}(n-1)^2 = k^2 + (n-1)k,$$

satisfies

$$(4.39) \quad \dim V_k = \frac{2k+n-1}{n-1} \binom{k+n-2}{k} = \binom{k+n-2}{k-1} + \binom{k+n-1}{k}.$$

In particular, on S^2 we have $\dim V_k = 2k + 1$.

Another natural approach to E_k is via the wave equation. We have

$$(4.40) \quad \begin{aligned} E_k &= \frac{1}{2T} \int_{-T}^T e^{-iv_k t} e^{itA} dt \\ &= \frac{1}{2T} \int_{-T}^T \cos t(A - v_k) dt, \end{aligned}$$

where $T = \pi$ or 2π depending on whether n is odd or even. (In either case, one can take $T = 2\pi$.) In the special case of S^2 , when (4.18) is used, comparison of (4.36) with the formula produced by this method produces the identity

$$(4.41) \quad P_k(\cos \theta) = \frac{1}{\pi} \int_{-\theta}^{\theta} \frac{\cos(k + \frac{1}{2})t}{(2 \cos t - 2 \cos \theta)^{1/2}} dt,$$

for the Legendre polynomials, known as the *Mehler-Dirichlet formula*.

Exercises

Exercises 1–5 deal with results that follow from symmetries of the sphere. The group $\mathrm{SO}(n+1)$ acts as a group of isometries of $S^n \subset \mathbb{R}^{n+1}$, hence as a group of unitary operators on $L^2(S^n)$. Each eigenspace V_k of the Laplace operator is preserved by this action. Fix $p = (0, \dots, 0, 1) \in S^n$, regarded as the “north pole.” The subgroup of $\mathrm{SO}(n+1)$ fixing p is a copy of $\mathrm{SO}(n)$.

1. Show that each eigenspace V_k has an element u such that $u(p) \neq 0$. Conclude by forming

$$\int_{\mathrm{SO}(n)} u(gx) dg$$

that each eigenspace V_k of Δ_S has an element $z_k \neq 0$ such that $z_k(x) = z_k(gx)$, for all $g \in \mathrm{SO}(n)$. Such a function is called a *spherical function*.

2. Suppose V_k has a proper subspace W invariant under $\mathrm{SO}(n+1)$. (Hence $W^\perp \subset V_k$ is also invariant.) Show that W must contain a nonzero spherical function.
3. Suppose z_k and y_k are two nonzero spherical functions in V_k . Show that they must be multiples of each other. Hence the unique spherical functions (up to constant multiples) are given by (4.35), with $y = p$. (Hint: z_k and y_k are eigenfunctions of $-\Delta_S$, with eigenvalue $\lambda_k = k^2 + (n-1)k$. Pick a sequence of surfaces

$$\Sigma_j = \{x \in S^n : \theta(x, p) = \varepsilon_j\} \subset S^n,$$

with $\varepsilon_j \rightarrow 0$, on which $z_k = \alpha_j \neq 0$. With $\beta_j = y_k|_{\Sigma_j}$, it follows that $\beta_j z_k - \alpha_j y_k$ is an eigenfunction of $-\Delta_S$ that vanishes on Σ_j . Show that, for j large, this forces $\beta_j z_k - \alpha_j y_k$ to be identically zero.)

4. Using Exercises 2 and 3, show that the action of $\mathrm{SO}(n+1)$ on each eigenspace V_k is irreducible, that is, V_k has no proper invariant subspaces.
5. Show that each V_k is equal to the linear span of the set of polynomials of the form $p_c(x) = (c_1 x_1 + \dots + c_{n+1} x_{n+1})^k$, with $\langle c, c \rangle = 0$. (Hint: Show that this linear span is invariant under $\mathrm{SO}(n+1)$.)
6. Using (4.9), show that

$$(4.42) \quad \mathrm{Tr} e^{-tA} = \frac{2 \sinh t}{(2 \cosh t - 2)^{(n+1)/2}}.$$

Find the asymptotic behavior as $t \searrow 0$. Use Karamata's Tauberian theorem to determine the asymptotic behavior of the eigenvalues of A , hence of $-\Delta_S$. Compare this with the general results of §3 and also with the explicit results of Corollary 4.3.

7. Using (4.27), show that, for A on S^n with $n = 2k + 1$,

$$(4.43) \quad \begin{aligned} \mathrm{Tr} e^{-tA^2} &= \frac{A_{2k+1}}{\sqrt{4\pi t}} \left(-\frac{1}{2\pi} \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \right)^k e^{-\theta^2/4t} \Big|_{\theta=0} + O(t^\infty) \\ &= (4\pi t)^{-n/2} A_{2k+1} + O(t^{-n/2+1}), \end{aligned}$$

as $t \searrow 0$. Compare the general results of §3.

8. Show that

$$(4.44) \quad e^{-\pi i(A-(n-1)/2)} f(\omega) = f(-\omega), \quad f \in L^2(S^n).$$

(Hint: Check it for $f \in V_k$, the restriction to S^n of a homogeneous harmonic polynomial of degree k .)

Exercises 9–13 deal with analysis on S^n when $n = 2$. When doing them, look for generalizations to other values of n .

9. If $\Xi(A)$ has integral kernel $K_\Xi(x, y)$, show that when $n = 2$,

$$(4.45) \quad K_\Xi(x, y) = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} (2\ell+1) \Xi\left(\ell + \frac{1}{2}\right) P_\ell(\cos \theta),$$

where $\cos \theta = x \cdot y$ and $P_\ell(t)$ are the Legendre polynomials.

10. Demonstrate the Rodrigues formula for the Legendre polynomials:

$$(4.46) \quad P_k(t) = \frac{1}{2^k k!} \left(\frac{d}{dt}\right)^k (t^2 - 1)^k.$$

(Hint: Use Cauchy's formula to get

$$P_k(t) = \frac{1}{2\pi i} \int_{\gamma} (1 - 2zt + z^2)^{-1/2} z^{-k-1} dz$$

from (4.33); then use the change of variable $1 - uz = (1 - 2tz + z^2)^{1/2}$. Then appeal to Cauchy's formula again, to analyze the resulting integral.)

11. If $f \in L^2(S^2)$ has the form $f(x) = g(x \cdot y) = \sum \varphi_\ell P_\ell(x \cdot y)$, for some $y \in S^2$, show that

$$(4.47) \quad \varphi_\ell = \frac{2\ell+1}{4\pi} \int_{S^2} f(z) P_\ell(y \cdot z) dS(z) = \left(\ell + \frac{1}{2}\right) \int_{-1}^1 g(t) P_\ell(t) dt.$$

(Hint: Use $\int_{S^2} E_k(x, z) E_\ell(z, y) dS(z) = \delta_{k\ell} E_\ell(x, y)$.) Conclude that $g(x \cdot y)$ is the integral kernel of $\psi(A - 1/2)$, where

$$(4.48) \quad \psi(\ell) = \frac{4\pi}{2\ell+1} \varphi_\ell = 2\pi \int_{-1}^1 g(t) P_\ell(t) dt.$$

This result is known as the Funk-Hecke theorem.

12. Show that, for $x, y \in S^2$,

$$(4.49) \quad e^{ikx \cdot y} = \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell j_\ell(k) P_\ell(x \cdot y),$$

where

$$(4.50) \quad j_\ell(z) = \left(\frac{\pi}{2z}\right)^{1/2} J_{\ell+1/2}(z) = \frac{1}{2} \frac{1}{\ell!} \left(\frac{z}{2}\right)^\ell \int_{-1}^1 (1-t^2)^\ell e^{izt} dt.$$

(Hint: Take $g(t) = e^{ikt}$ in Exercise 11, apply the Rodrigues formula, and integrate by parts.) Thus $e^{ikx \cdot y}$ is the integral kernel of the operator

$$4\pi e^{(1/2)\pi i(A-1/2)} j_{A-1/2}(k)$$

For another approach, see Exercises 10 and 11 in §9 of Chap. 9.

13. Demonstrate the identities

$$(4.51) \quad \left[(1-t^2) \frac{d}{dt} + \ell t \right] P_\ell(t) = \ell P_{\ell-1}(t)$$

and

$$(4.52) \quad \frac{d}{dt} \left[(1-t^2) \frac{d}{dt} P_\ell(t) \right] + \ell(\ell+1) P_\ell(t) = 0.$$

Relate (4.52) to the statement that, for fixed $y \in S^2$, $\varphi(x) = P_\ell(x \cdot y)$ belongs to the $\ell(\ell+1)$ -eigenspace of $-\Delta_S$.

Exercises 14–19 deal with formulas for an orthogonal basis of V_k (for S^2). We will make use of the structure of irreducible representations of $\text{SO}(3)$, obtained in §9 of Appendix B, Manifolds, Vector Bundles, and Lie Groups.

14. Show that the representation of $\text{SO}(3)$ on V_k is equivalent to the representation D_k , for each $k = 0, 1, 2, \dots$

15. Show that if we use coordinates (θ, ψ) on S^2 , where θ is the geodesic distance from $(1, 0, 0)$ and ψ is the angular coordinate about the x_1 -axis in \mathbb{R}^3 , then

$$(4.53) \quad L_1 = \frac{\partial}{\partial \psi}, \quad L_\pm = i e^{\pm i \psi} \left[\pm \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \psi} \right].$$

16. Set

$$(4.54) \quad w_k(x) = (x_2 + i x_3)^k = \sin^k \theta e^{i k \psi}.$$

Show that $w_k \in V_k$ and that it is the highest-weight vector for the representation, so

$$L_1 w_k = i k w_k$$

17. Show that an orthogonal basis of V_k is given by

$$w_k, L_- w_k, \dots, L_-^{2k} w_k$$

18. Show that the functions $\zeta_{kj} = L_-^{k-j} w_k$, $j \in \{-k, -k+1, \dots, k-1, k\}$, listed in Exercise 17 coincide, up to nonzero constant factors, with z_{kj} , given by

$$z_{k0} = z_k,$$

the spherical function considered in Exercises 1–3, and, for $1 \leq j \leq k$,

$$z_{k,-j} = L_-^j z_k, \quad z_{kj} = L_+^j z_k$$

19. Show that the functions z_{kj} coincide, up to nonzero constant factors, with

$$(4.55) \quad e^{i j \psi} P_k^j(\cos \theta), \quad -k \leq j \leq k,$$

where $P_k^j(t)$, called *associated Legendre functions*, are defined by

$$(4.56) \quad P_k^j(t) = (-1)^j (1-t^2)^{|j|/2} \left(\frac{d}{dt} \right)^{|j|} P_k(t).$$

5. The Laplace operator on hyperbolic space

The hyperbolic space \mathcal{H}^n shares with the sphere S^n the property of having constant sectional curvature, but for \mathcal{H}^n it is -1 . One way to describe \mathcal{H}^n is as a set of vectors with square length 1 in \mathbb{R}^{n+1} , not for a Euclidean metric, but rather for a Lorentz metric

$$(5.1) \quad \langle v, v \rangle = -v_1^2 - \cdots - v_n^2 + v_{n+1}^2,$$

namely,

$$(5.2) \quad \mathcal{H}^n = \{v \in \mathbb{R}^{n+1} : \langle v, v \rangle = 1, v_{n+1} > 0\},$$

with metric tensor induced from (5.1). The connected component G of the identity of the group $O(n, 1)$ of linear transformations preserving the quadratic form (5.1) acts transitively on \mathcal{H}^n , as a group of isometries. In fact, $SO(n)$, acting on $\mathbb{R}^n \subset \mathbb{R}^{n+1}$, leaves invariant $p = (0, \dots, 0, 1) \in \mathcal{H}^n$ and acts transitively on the unit sphere in $T_p \mathcal{H}^n$. Also, if $A(u_1, \dots, u_n, u_{n+1})^t = (u_1, \dots, u_{n+1}, u_n)^t$, then e^{tA} is a one-parameter subgroup of $SO(n, 1)$ taking p to the curve

$$\gamma = \{(0, \dots, 0, x_n, x_{n+1}) : x_{n+1}^2 - x_n^2 = 1, x_{n+1} > 0\}$$

Together these facts imply that \mathcal{H}^n is a homogeneous space.

There is a map of \mathcal{H}^n onto the unit ball in \mathbb{R}^n , defined in a fashion similar to the stereographic projection of S^n . The map

$$(5.3) \quad \mathfrak{s} : \mathcal{H}^n \longrightarrow B^n = \{x \in \mathbb{R}^n : |x| < 1\}$$

is defined by

$$(5.4) \quad \mathfrak{s}(x, x_{n+1}) = (1 + x_{n+1})^{-1}x.$$

The metric on \mathcal{H}^n defined above then yields the following metric tensor on B^n :

$$(5.5) \quad ds^2 = 4(1 - |x|^2)^{-2} \sum_{j=1}^n dx_j^2.$$

Another useful representation of hyperbolic space is as the upper half space $\mathbb{R}_+^n = \{x \in \mathbb{R}^n : x_n > 0\}$, with a metric we will specify shortly. In fact, with $e_n = (0, \dots, 0, 1)$,

$$(5.6) \quad \tau(x) = |x + e_n|^{-2}(x + e_n) - \frac{1}{2}e_n$$

defines a map of the unit ball B^n onto \mathbb{R}_+^n , taking the metric (5.5) to

$$(5.7) \quad ds^2 = x_n^{-2} \sum_{j=1}^n dx_j^2.$$

The Laplace operator for the metric (5.7) has the form

$$\begin{aligned}
 \Delta u &= \sum_{j=1}^n x_n^n \partial_j (x_n^{2-n} \partial_j u) \\
 (5.8) \quad &= x_n^2 \sum_{j=1}^n \partial_j^2 u + (2-n)x_n \partial_n u.
 \end{aligned}$$

which is convenient for a number of computations, such as (5.9) in the following:

Proposition 5.1. *If Δ is the Laplace operator on \mathcal{H}^n , then Δ is essentially self-adjoint on $C_0^\infty(\mathcal{H}^n)$, and its natural self-adjoint extension has the property*

$$(5.9) \quad \text{spec}(-\Delta) \subset \left[\frac{1}{4}(n-1)^2, \infty \right).$$

Proof. Since \mathcal{H}^n is a complete Riemannian manifold, the essential self-adjointness on $C_0^\infty(\mathcal{H}^n)$ follows from Proposition 2.4. To establish (5.9), it suffices to show that

$$(-\Delta u, u)_{L^2(\mathcal{H}^n)} \geq \frac{(n-1)^2}{4} \|u\|_{L^2(\mathcal{H}^n)}^2,$$

for all $u \in C_0^\infty(\mathcal{H}^n)$. Now the volume element on \mathcal{H}^n , identified with the upper half-space with the metric (5.7), is $x_n^{-n} dx_1 \cdots dx_n$, so for such u we have

$$\begin{aligned}
 &\left(\left(-\Delta - \frac{1}{4}(n-1)^2 \right) u, u \right)_{L^2} \\
 (5.10) \quad &= \int \left[(\partial_n u)^2 - \left(\frac{(n-1)u}{2x_n} \right)^2 \right] x_n^{2-n} dx_1 \cdots dx_n \\
 &\quad + \sum_{j=1}^{n-1} \int (\partial_j u)^2 x_n^{2-n} dx_1 \cdots dx_n.
 \end{aligned}$$

Now, by an integration by parts, the first integral on the right is equal to

$$(5.11) \quad \int_{\mathbb{R}_+^n} \left[\partial_n (x_n^{-(n-1)/2} u) \right]^2 x_n dx_1 \cdots dx_n.$$

Thus the expression (5.10) is ≥ 0 , and (5.9) is proved.

We next describe how to obtain the fundamental solution to the wave equation on \mathcal{H}^n . This will be obtained from the formula for S^n , via an analytic continuation in the metric tensor. Let p be a fixed point (e.g., the north pole) in S^n , taken to be the origin in geodesic normal coordinates. Consider the one-parameter family of metrics given by dilating the sphere, which has constant curvature $K = 1$. Spheres dilated to have radius > 1 have constant curvature $K \in (0, 1)$. On such a space, the fundamental kernel $A^{-1} \sin t A \delta_p(x)$, with

$$(5.12) \quad A = \left(-\Delta + \frac{K}{4}(n-1)^2 \right)^{1/2},$$

can be obtained explicitly from that on the unit sphere by a change of scale. The explicit representation so obtained continues analytically to all real values of K and at $K = -1$ gives a formula for the wave kernel,

$$(5.13) \quad A^{-1} \sin t A \delta_p(x) = R(t, p, x), \quad A = \left(-\Delta - \frac{1}{4}(n-1)^2 \right)^{1/2}.$$

We have

$$(5.14) \quad R(t, p, x) = \lim_{\varepsilon \searrow 0} -2C_n \operatorname{Im} [2 \cos(it - \varepsilon) - 2 \cosh r]^{-(n-1)/2},$$

where $r = r(p, x)$ is the geodesic distance from p to x . Here, as in (4.10), $C_n = 1/(n-1)A_n$. This exhibits several properties similar to those in the case of S^n discussed in §4. Of course, for $r > |t|$, the limit vanishes, exhibiting the finite propagation speed phenomenon. Also, if n is odd, the exponent $(n-1)/2$ is an integer, which implies that (5.14) is supported on the shell $r = |t|$.

In analogy with (4.25), we have the following formula for $g(A)\delta_p(x)$, for $g \in S(\mathbb{R})$, when acting on $L^2(\mathcal{H}^n)$, with $n = 2k + 1$:

$$(5.15) \quad g(A) = (2\pi)^{-1/2} \left(-\frac{1}{2\pi} \frac{1}{\sinh r} \frac{\partial}{\partial r} \right)^k \hat{g}(r).$$

If $n = 2k$, we have

$$(5.16) \quad \frac{1}{\pi^{1/2}} \int_r^\infty \left(-\frac{1}{2\pi} \frac{1}{\sinh s} \frac{\partial}{\partial s} \right)^k \hat{g}(s) (\cosh s - \cosh r)^{-1/2} \sinh s \, ds.$$

Exercises

1. If $n = 2k + 1$, show that the Schwartz kernel of $(-\Delta - (n-1)^2/4 - z^2)^{-1}$ on \mathcal{H}^n , for $z \in \mathbb{C} \setminus [0, \infty)$, is

$$G_z(x, y) = -\frac{1}{2iz} \left(-\frac{1}{2\pi} \frac{1}{\sinh r} \frac{\partial}{\partial r} \right)^k e^{izr},$$

where $r = r(x, y)$ is geodesic distance, and the integral kernel of $e^{t(\Delta + (n-1)^2/4)}$, for $t > 0$, is

$$H_t(x, y) = \frac{1}{\sqrt{4\pi t}} \left(-\frac{1}{2\pi} \frac{1}{\sinh r} \frac{\partial}{\partial r} \right)^k e^{-r^2/4t}$$

6. The harmonic oscillator

We consider the differential operator $H = -\Delta + |x|^2$ on $L^2(\mathbb{R}^n)$. By Proposition 2.7, H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. Furthermore, as a special case of Proposition 2.8, we know that H has compact resolvent, so $L^2(\mathbb{R}^n)$ has an orthonormal basis of eigenfunctions of H . To work out the spectrum, it suffices to work with the case $n = 1$, so we consider $H = D^2 + x^2$, where $D = -i d/dx$.

The spectral analysis follows by some simple algebraic relations, involving the operators

$$(6.1) \quad \begin{aligned} a &= D - ix = \frac{1}{i} \left(\frac{d}{dx} + x \right), \\ a^+ &= D + ix = \frac{1}{i} \left(\frac{d}{dx} - x \right). \end{aligned}$$

Note that on $\mathcal{D}'(\mathbb{R})$,

$$(6.2) \quad H = aa^+ - I = a^+a + I,$$

and

$$(6.3) \quad [H, a] = -2a, \quad [H, a^+] = 2a^+.$$

Suppose that $u_j \in C^\infty(\mathbb{R})$ is an eigenfunction of H , that is,

$$(6.4) \quad u_j \in \mathcal{D}(H), \quad Hu_j = \lambda_j u_j.$$

Now, by material developed in §2,

$$(6.5) \quad \begin{aligned} \mathcal{D}(H^{1/2}) &= \{u \in L^2(\mathbb{R}) : Du \in L^2(\mathbb{R}), xu \in L^2(\mathbb{R})\}, \\ \mathcal{D}(H) &= \{u \in L^2(\mathbb{R}) : D^2u + x^2u \in L^2(\mathbb{R})\}. \end{aligned}$$

Since certainly each u_j belongs to $\mathcal{D}(H^{1/2})$, it follows that au_j and a^+u_j belong to $L^2(\mathbb{R})$. By (6.3), we have

$$(6.6) \quad H(au_j) = (\lambda_j - 2)au_j, \quad H(a^+u_j) = (\lambda_j + 2)a^+u_j.$$

It follows that au_j and a^+u_j belong to $\mathcal{D}(H)$ and are eigenfunctions. Hence, if

$$(6.7) \quad \text{Eigen}(\lambda, H) = \{u \in \mathcal{D}(H) : Hu = \lambda u\},$$

we have, for all $\lambda \in \mathbb{R}$,

$$(6.8) \quad \begin{aligned} a^+ : \text{Eigen}(\lambda, H) &\rightarrow \text{Eigen}(\lambda + 2, H), \\ a : \text{Eigen}(\lambda + 2, H) &\rightarrow \text{Eigen}(\lambda, H). \end{aligned}$$

From (6.2) it follows that $(Hu, u) \geq \|u\|_{L^2}^2$, for all $u \in C_0^\infty(\mathbb{R})$; hence, in view of essential self-adjointness,

$$(6.9) \quad \text{spec } H \subset [1, \infty), \quad \text{for } n = 1.$$

Now each space $\text{Eigen}(\lambda, H)$ is a finite-dimensional subspace of $C^\infty(\mathbb{R})$, and, by (6.2), we conclude that, in (6.8), a^+ is an isomorphism of $\text{Eigen}(\lambda_j, H)$ onto $\text{Eigen}(\lambda_j + 2, H)$, for each $\lambda_j \in \text{spec } H$. Also, a is an isomorphism of $\text{Eigen}(\lambda_j, H)$ onto $\text{Eigen}(\lambda_j - 2, H)$, for all $\lambda_j > 1$. On the other hand, a must annihilate $\text{Eigen}(\lambda_0, H)$ when λ_0 is the smallest element of $\text{spec } H$, so

$$(6.10) \quad \begin{aligned} u_0 \in \text{Eigen}(\lambda_0, H) &\implies u_0'(x) = -xu_0(x) \\ &\implies u_0(x) = K e^{-x^2/2}. \end{aligned}$$

Thus

$$(6.11) \quad \lambda_0 = 1, \quad \text{Eigen}(1, H) = \text{span}(e^{-x^2/2}).$$

Since $e^{-x^2/2}$ spans the null space of a , acting on $C^\infty(\mathbb{R})$, and since each nonzero space $\text{Eigen}(\lambda_j, H)$ is mapped by some power of a to this null space, it follows that, for $n = 1$,

$$(6.12) \quad \text{spec } H = \{2k + 1 : k = 0, 1, 2, \dots\}$$

and

$$(6.13) \quad \text{Eigen}(2k + 1, H) = \text{span} \left(\left(\frac{\partial}{\partial x} - x \right)^k e^{-x^2/2} \right).$$

One also writes

$$(6.14) \quad \left(\frac{\partial}{\partial x} - x \right)^k e^{-x^2/2} = H_k(x) e^{-x^2/2},$$

where $H_k(x)$ are the *Hermite polynomials*, given by

$$(6.15) \quad \begin{aligned} H_k(x) &= (-1)^k e^{x^2} \left(\frac{d}{dx} \right)^k e^{-x^2} \\ &= \sum_{j=0}^{[k/2]} (-1)^j \frac{k!}{j!(k-2j)!} (2x)^{k-2j}. \end{aligned}$$

We define eigenfunctions of H :

$$(6.16) \quad h_k(x) = c_k \left(\frac{\partial}{\partial x} - x \right)^k e^{-x^2/2} = c_k H_k(x) e^{-x^2/2},$$

where c_k is the unique positive number such that $\|h_k\|_{L^2(\mathbb{R})} = 1$. To evaluate c_k , note that

$$(6.17) \quad \|a^+ h_k\|_{L^2}^2 = (aa^+ h_k, h_k)_{L^2} = 2(k+1) \|h_k\|_{L^2}^2.$$

Thus, if $\|h_k\|_{L^2} = 1$, in order for $h_{k+1} = \gamma_k a^+ h_k$ to have unit norm, we need $\gamma_k = (2k+2)^{-1/2}$. Hence

$$(6.18) \quad c_k = [\pi^{1/2} 2^k (k!)]^{-1/2}.$$

Of course, given the analysis above of H on $L^2(\mathbb{R})$, then for $H = -\Delta + |x|^2$ on $L^2(\mathbb{R}^n)$, we have

$$(6.19) \quad \text{spec } H = \{2k + n : k = 0, 1, 2, \dots\}.$$

In this case, an orthonormal basis of $\text{Eig}(2k + n, H)$ is given by

$$(6.20) \quad c_{k_1} \cdots c_{k_n} H_{k_1}(x_1) \cdots H_{k_n}(x_n) e^{-|x|^2/2}, \quad k_1 + \cdots + k_n = k,$$

where $k_v \in \{0, \dots, k\}$, the $H_{k_v}(x_v)$ are the Hermite polynomials, and the c_{k_v} are given by (6.18). The dimension of this eigenspace is the same as the dimension of the space of homogeneous polynomials of degree k in n variables.

We now want to derive a formula for the semigroup e^{-tH} , $t > 0$, called the *Hermite semigroup*. Again it suffices to treat the case $n = 1$. To some degree paralleling the analysis of the eigenfunctions above, we can produce this formula via some commutator identities, involving the operators

$$(6.21) \quad X = D^2 = -\partial_x^2, \quad Y = x^2, \quad Z = x\partial_x + \partial_x x = 2x\partial_x + 1.$$

Note that $H = X + Y$. The commutator identities are

$$(6.22) \quad [X, Y] = -2Z, \quad [X, Z] = 4X, \quad [Y, Z] = -4Y.$$

Thus, X, Y , and Z span a three-dimensional, real Lie algebra. This is isomorphic to $\mathfrak{sl}(2, \mathbb{R})$, the Lie algebra consisting of 2×2 real matrices of trace zero, spanned by

$$(6.23) \quad n_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad n_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \alpha = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We have

$$(6.24) \quad [n_+, n_-] = \alpha, \quad [n_+, \alpha] = -2n_+, \quad [n_-, \alpha] = 2n_-.$$

The isomorphism is implemented by

$$(6.25) \quad X \leftrightarrow 2n_+, \quad Y \leftrightarrow 2n_-, \quad Z \leftrightarrow -2\alpha.$$

Now we will be able to write

$$(6.26) \quad e^{-t(2n_++2n_-)} = e^{-2\sigma_1(t)n_+} e^{-2\sigma_3(t)\alpha} e^{-2\sigma_2(t)n_-},$$

as we will see shortly, and, once this is accomplished, we will be motivated to suspect that also

$$(6.27) \quad e^{-tH} = e^{-\sigma_1(t)X} e^{\sigma_3(t)Z} e^{-\sigma_2(t)Y}.$$

To achieve (6.26), write

$$(6.28) \quad \begin{aligned} e^{-2\sigma_1 n_+} &= \begin{pmatrix} 1 & -2\sigma_1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & x \\ 0 & 1 \end{pmatrix}, \\ e^{-2\sigma_3 \alpha} &= \begin{pmatrix} e^{-2\sigma_3} & 0 \\ 0 & e^{2\sigma_3} \end{pmatrix} = \begin{pmatrix} y & 0 \\ 0 & 1/y \end{pmatrix}, \\ e^{-2\sigma_2 n_-} &= \begin{pmatrix} 1 & 0 \\ -2\sigma_2 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ z & 1 \end{pmatrix}, \end{aligned}$$

and

$$(6.29) \quad e^{-2t(n_++n_-)} = \begin{pmatrix} \cosh 2t & -\sinh 2t \\ -\sinh 2t & \cosh 2t \end{pmatrix} = \begin{pmatrix} u & v \\ v & u \end{pmatrix}.$$

Then (6.26) holds if and only if

$$(6.30) \quad y = \frac{1}{u} = \frac{1}{\cosh 2t}, \quad x = z = \frac{v}{u} = -\tanh 2t,$$

so the quantities $\sigma_j(t)$ are given by

$$(6.31) \quad \sigma_1(t) = \sigma_2(t) = \frac{1}{2} \tanh 2t, \quad e^{2\sigma_3(t)} = \cosh 2t.$$

Now we can compute the right side of (6.27). Note that

$$\begin{aligned}
 e^{-\sigma_1 X} u(x) &= (4\pi\sigma_1)^{-1/2} \int e^{-(x-y)^2/4\sigma_1} u(y) dy, \\
 e^{-\sigma_2 Y} u(x) &= e^{-\sigma_2 x^2} u(x), \\
 e^{\sigma_3 Z} u(x) &= e^{\sigma_3} u(e^{2\sigma_3} x).
 \end{aligned}
 \tag{6.32}$$

Upon composing these operators we find that, for $n = 1$,

$$e^{-tH} u(x) = \int K_t(x, y) u(y) dy, \tag{6.33}$$

with

$$K_t(x, y) = \frac{\exp\left\{\left[-\frac{1}{2}(\cosh 2t)(x^2 + y^2) + xy\right]/\sinh 2t\right\}}{(2\pi \sinh 2t)^{1/2}}. \tag{6.34}$$

This is known as Mehler's formula for the Hermite semigroup. Clearly, for general n , we have

$$e^{-tH} u(x) = \int K_n(t, x, y) u(y) dy, \tag{6.35}$$

with

$$K_n(t, x, y) = K_t(x_1, y_1) \cdots K_t(x_n, y_n). \tag{6.36}$$

The idea behind passing from (6.26) to (6.27) is that the Lie algebra homomorphism defined by (6.25) should give rise to a Lie group homomorphism from (perhaps a covering group G of) $\mathrm{SL}(2, \mathbb{R})$ into a group of operators. Since this involves an infinite-dimensional representation of G (not necessarily by bounded operators here, since e^{-tH} is bounded only for $t \geq 0$), there are analytical problems that must be overcome to justify this reasoning. Rather than take the space to develop such analysis here, we will instead just give a direct justification of (6.33)–(6.34).

Indeed, let $v(t, x)$ denote the right side of (6.33), with $u \in L^2(\mathbb{R})$ given. The rapid decrease of $K_t(x, y)$ as $|x| + |y| \rightarrow \infty$, for $t > 0$, makes it easy to show that

$$u \in L^2(\mathbb{R}) \implies v \in C^\infty((0, \infty), \mathcal{S}(\mathbb{R})). \tag{6.37}$$

Also, it is routine to verify that

$$\frac{\partial v}{\partial t} = -Hv. \tag{6.38}$$

Simple estimates yielding uniqueness then imply that, for each $s > 0$,

$$(6.39) \quad v(t + s, \cdot) = e^{-tH} v(s, \cdot).$$

Indeed, if $w(t, \cdot)$ denotes the difference between the two sides of (6.39), then we have $w(0) = 0$, $w \in C(\mathbb{R}^+, \mathcal{D}(H))$, $\partial w / \partial t \in C(\mathbb{R}^+, L^2(\mathbb{R}))$, and

$$\frac{d}{dt} \|w(t)\|_{L^2}^2 = -2(Hw, w) \leq 0,$$

so $w(t) = 0$, for all $t \geq 0$.

Finally, as $t \searrow 0$, we see from (6.31) that each $\sigma_j(t) \searrow 0$. Since $v(t, x)$ is also given by the right side of (6.27), we conclude that

$$(6.40) \quad v(t, \cdot) \rightarrow u \text{ in } L^2(\mathbb{R}), \text{ as } t \searrow 0.$$

Thus we can let $s \searrow 0$ in (6.39), obtaining a complete proof that $e^{-tH}u$ is given by (6.33) when $n = 1$.

It is useful to write down the formula for e^{-tH} using the Weyl calculus, introduced in §14 of Chap. 7. We recall that it associates to $a(x, \xi)$ the operator

$$(6.41) \quad \begin{aligned} a(X, D)u &= (2\pi)^{-n} \int \hat{a}(q, p) e^{i(q \cdot X + p \cdot D)} u(x) \, dq \, dp \\ &= (2\pi)^{-n} \int a\left(\frac{x+y}{2}, \xi\right) e^{i(x-y) \cdot \xi} u(y) \, dy \, d\xi. \end{aligned}$$

In other words, the operator $a(X, D)$ has integral kernel $K_a(x, y)$, for which

$$a(X, D)u(x) = \int K_a(x, y) u(y) \, dy,$$

given by

$$K_a(x, y) = (2\pi)^{-n} \int a\left(\frac{x+y}{2}, \xi\right) e^{i(x-y) \cdot \xi} \, d\xi$$

Recovery of $a(x, \xi)$ from $K_a(x, y)$ is an exercise in Fourier analysis. When it is applied to the formulas (6.33)–(6.36), this exercise involves computing a Gaussian integral, and we obtain the formula

$$(6.42) \quad e^{-tH} = h_t(X, D)$$

on $L^2(\mathbb{R}^n)$, with

$$(6.43) \quad h_t(x, \xi) = (\cosh t)^{-n} e^{-(\tanh t)(|x|^2 + |\xi|^2)}.$$

It is interesting that this formula, while equivalent to (6.33)–(6.36), has a simpler and more symmetrical appearance.

In fact, the formula (6.43) was derived in §15 of Chap. 7, by a different method, which we briefly recall here. For reasons of symmetry, involving the identity (14.19), one can write

$$(6.44) \quad h_t(x, \xi) = g(t, Q), \quad Q(x, \xi) = |x|^2 + |\xi|^2.$$

Note that (6.42) gives $\partial_t h_t(X, D) = -H h_t(X, D)$. Now the composition formula for the Weyl calculus implies that $h_t(x, \xi)$ satisfies the following evolution equation:

$$(6.45) \quad \begin{aligned} \frac{\partial}{\partial t} h_t(x, \xi) &= -(Q \circ h_t)(x, \xi) \\ &= -Q(x, \xi) h_t(x, \xi) - \frac{1}{2} \{Q, h_t\}_2(x, \xi) \\ &= -(|x|^2 + |\xi|^2) h_t(x, \xi) + \frac{1}{4} \sum_k (\partial_{x_k}^2 + \partial_{\xi_k}^2) h_t(x, \xi). \end{aligned}$$

Given (6.44), we have for $g(t, Q)$ the equation

$$(6.46) \quad \frac{\partial g}{\partial t} = -Qg + Q \frac{\partial^2 g}{\partial Q^2} + n \frac{\partial g}{\partial Q}.$$

It is easy to verify that (6.43) solves this evolution equation, with $h_0(x, \xi) = 1$.

We can obtain a formula for

$$(6.47) \quad e^{-tQ(X, D)} = h_t^Q(X, D),$$

for a general positive-definite quadratic form $Q(x, \xi)$. First, in the case

$$(6.48) \quad Q(x, \xi) = \sum_{j=1}^n \mu_j (x_j^2 + \xi_j^2), \quad \mu_j > 0,$$

it follows easily from (6.43) and multiplicativity, as in (6.36), that

$$(6.49) \quad h_t^Q(x, \xi) = \prod_{j=1}^n (\cosh t\mu_j)^{-1} \cdot \exp \left\{ - \sum_{j=1}^n (\tanh t\mu_j) (x_j^2 + \xi_j^2) \right\}.$$

Now any positive quadratic form $Q(x, \xi)$ can be put in the form (6.48) via a linear symplectic transformation, so to get the general formula we need only rewrite (6.49) in a symplectically invariant fashion. This is accomplished using the “Hamilton map” F_Q , a skew-symmetric transformation on \mathbb{R}^{2n} defined by

$$(6.50) \quad Q(u, v) = \sigma(u, F_Q v), \quad u, v \in \mathbb{R}^{2n},$$

where $Q(u, v)$ is the bilinear form polarizing Q , and σ is the symplectic form on \mathbb{R}^{2n} ; $\sigma(u, v) = x \cdot \xi' - x' \cdot \xi$ if $u = (x, \xi)$, $v = (x', \xi')$. When Q has the form (6.48), F_Q is a sum of 2×2 blocks $\begin{pmatrix} 0 & \mu_j \\ -\mu_j & 0 \end{pmatrix}$, and we have

$$(6.51) \quad \prod_{j=1}^n (\cosh t\mu_j)^{-1} = \left(\det \cosh itF_Q \right)^{-1/2}.$$

Passing from F_Q to

$$(6.52) \quad A_Q = (-F_Q^2)^{1/2},$$

the unique positive-definite square root, means passing to blocks

$$\begin{pmatrix} \mu_j & 0 \\ 0 & \mu_j \end{pmatrix},$$

and when Q has the form (6.48), then

$$(6.53) \quad \sum_{j=1}^n (\tanh t\mu_j)(x_j^2 + \xi_j^2) = tQ(\vartheta(tA_Q)\zeta, \zeta),$$

where $\zeta = (x, \xi)$ and

$$(6.54) \quad \vartheta(t) = \frac{\tanh t}{t}.$$

Thus the general formula for (6.47) is

$$(6.55) \quad h_t^Q(x, \xi) = \left(\cosh tA_Q \right)^{-1/2} e^{-tQ(\vartheta(tA_Q)\zeta, \zeta)}.$$

Exercises

1. Define an unbounded operator A on $L^2(\mathbb{R})$ by

$$\mathcal{D}(A) = \{u \in L^2(\mathbb{R}) : Du \in L^2(\mathbb{R}), xu \in L^2(\mathbb{R})\}, \quad Au = Du - i xu.$$

Show that A is closed and that the self-adjoint operator H satisfies

$$H = A^*A + I = AA^* - I$$

(Hint: Note Exercises 5–7 of §2.)

2. If $H_k(x)$ are the Hermite polynomials, show that there is the generating function identity

$$\sum_{k=0}^{\infty} \frac{1}{k!} H_k(x) s^k = e^{2xs-s^2}$$

(Hint: Use the first identity in (6.15).)

3. Show that Mehler's formula (6.34) is equivalent to the identity

$$\sum_{j=0}^{\infty} h_j(x) h_j(y) s^j = \pi^{-1/2} (1-s^2)^{-1/2} \exp \left\{ (1-s^2)^{-1} [2xy s - (x^2 + y^2) s^2] \right\} \cdot e^{-(x^2+y^2)/2},$$

for $0 \leq s < 1$. Deduce that

$$\sum_{j=0}^{\infty} H_j(x)^2 \frac{s^j}{2^j j!} = (1-s^2)^{-1/2} e^{2sx^2/(1+s)}, \quad |s| < 1.$$

4. Using

$$H^{-s} = \frac{1}{\Gamma(s)} \int_0^{\infty} e^{-tH} t^{s-1} dt, \quad \operatorname{Re} s > 0,$$

find the integral kernel $A_s(x, y)$ such that

$$H^{-s} u(x) = \int A_s(x, y) u(y) dy.$$

Writing $\operatorname{Tr} H^{-s} = \int A_s(x, x) dx$, $\operatorname{Re} s > 1$, $n = 1$, show that

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^{\infty} \frac{y^{s-1}}{e^y - 1} dy$$

See [Ing], pp. 41–44, for a derivation of the functional equation for the Riemann zeta function, using this formula.

5. Let $H_{\omega} = -d^2/dx^2 + \omega^2 x^2$. Show that $e^{-tH_{\omega}}$ has integral kernel

$$K_t^{\omega}(x, y) = (4\pi t)^{-1/2} \gamma(2\omega t)^{1/2} e^{-\gamma(2\omega t)[(\cosh 2\omega t)(x^2+y^2)-2xy]/4t},$$

where

$$\gamma(z) = \frac{z}{\sinh z}.$$

6. Consider the operator

$$\begin{aligned} Q(X, D) &= -\left(\frac{\partial}{\partial x_1} - i\omega x_2\right)^2 - \left(\frac{\partial}{\partial x_2} + i\omega x_1\right)^2 \\ &= -\Delta + \omega^2 |x|^2 + 2i\omega \left(x_2 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_2}\right). \end{aligned}$$

Note that $Q(x, \xi)$ is nonnegative, but not definite. Study the integral kernel $K_t^Q(x, y)$ of $e^{-tQ(X, D)}$. Show that

$$K_t^Q(x, 0) = (4\pi t)^{-1} \gamma(2\omega t) e^{-\tau(2\omega t)|x|^2/4t},$$

where

$$\tau(z) = z \coth z.$$

7. Let (ω_{jk}) be an invertible, $n \times n$, skew-symmetric matrix of real numbers (so n must be even). Suppose

$$L = - \sum_{j=1}^n \left(\frac{\partial}{\partial x_j} - i \sum_k \omega_{jk} x_k \right)^2.$$

Evaluate the integral kernel $K_L^L(x, y)$, particularly at $y = 0$.

8. In terms of the operators a, a^+ given by (6.1) and the basis of $L^2(\mathbb{R})$ given by (6.16)–(6.18), show that

$$a^+ h_k = \sqrt{2k+2} h_{k+1}, \quad a h_k = \sqrt{2k} h_{k-1}.$$

7. The quantum Coulomb problem

In this section we examine the operator

$$(7.1) \quad Hu = -\Delta u - K|x|^{-1}u,$$

acting on functions on \mathbb{R}^3 . Here, K is a positive constant.

This provides a quantum mechanical description of the Coulomb force between two charged particles. It is the first step toward a quantum mechanical description of the hydrogen atom, and it provides a decent approximation to the observed behavior of such an atom, though it leaves out a number of features. The most important omitted feature is the spin of the electron (and of the nucleus). Giving rise to further small corrections are the nonzero size of the proton, and relativistic effects, which confront one with great subtleties since relativity forces one to treat the electromagnetic field quantum mechanically. We refer to texts on quantum physics, such as [Mes], [Ser], [BLP], and [IZ], for work on these more sophisticated models of the hydrogen atom.

We want to define a self-adjoint operator via the Friedrichs method. Thus we want to work with a Hilbert space

$$(7.2) \quad \mathcal{H} = \left\{ u \in L^2(\mathbb{R}^3) : \nabla u \in L^2(\mathbb{R}^3), \int |x|^{-1} |u(x)|^2 dx < \infty \right\},$$

with inner product

$$(7.3) \quad (u, v)_{\mathcal{H}} = (\nabla u, \nabla v)_{L^2} + A(u, v)_{L^2} - K \int |x|^{-1} u(x) \overline{v(x)} dx,$$

where A is a sufficiently large, positive constant. We must first show that A can be picked to make this inner product positive-definite. In fact, we have the following:

Lemma 7.1. *For all $\varepsilon \in (0, 1]$, there exists $C(\varepsilon) < \infty$ such that*

$$(7.4) \quad \int |x|^{-1} |u(x)|^2 dx \leq \varepsilon \|\nabla u\|_{L^2}^2 + C(\varepsilon) \|u\|_{L^2}^2,$$

for all $u \in H^1(\mathbb{R}^3)$.

Proof. Here and below we will use the inclusion

$$(7.5) \quad H^s(\mathbb{R}^n) \subset L^p(\mathbb{R}^n), \quad \forall p \in \left[2, \frac{2n}{n-2s}\right), \quad 0 \leq s < \frac{n}{2},$$

from (2.42) of Chap. 4. In Chap. 13 we will establish the sharper result that $H^s(\mathbb{R}^n) \subset L^{2n/(n-2s)}(\mathbb{R}^n)$; for example, $H^1(\mathbb{R}^3) \subset L^6(\mathbb{R}^3)$. We will also cite this stronger result in some arguments below, though that could be avoided.

We also use the fact that (if $B = \{|x| < 1\}$ and $\chi_B(x)$ is its characteristic function),

$$\chi_B V \in L^q(\mathbb{R}^3), \quad \text{for all } q < 3$$

Here and below we will use $V(x) = |x|^{-1}$. Thus the left side of (7.4) is bounded by

$$(7.6) \quad \|\chi_B V\|_{L^q} \cdot \|u\|_{L^{2q'}}^2 + \|u\|_{L^2}^2 \leq C \|u\|_{H^\sigma(\mathbb{R}^3)}^2 + \|u\|_{L^2(\mathbb{R}^3)}^2,$$

where we can take any $q' > 3/2$; take $q' \in (3/2, 3)$. Then (7.6) holds for some $\sigma < 1$, for which $L^{2q'}(\mathbb{R}^3) \supset H^\sigma(\mathbb{R}^3)$. From this, (7.4) follows immediately.

Thus the Hilbert space \mathcal{H} in (7.2) is simply $H^1(\mathbb{R}^3)$, and we see that indeed, for some $A > 0$, (7.3) defines an inner product equivalent to the standard one on $H^1(\mathbb{R}^3)$. The Friedrichs method then defines a positive, self-adjoint operator $H + AI$, for which

$$(7.7) \quad \mathcal{D}((H + AI)^{1/2}) = H^1(\mathbb{R}^3).$$

Then

$$(7.8) \quad \mathcal{D}(H) = \{u \in H^1(\mathbb{R}^3) : -\Delta u - K|x|^{-1}u \in L^2(\mathbb{R}^3)\},$$

where $-\Delta u - K|x|^{-1}u$ is a priori regarded as an element of $H^{-1}(\mathbb{R}^3)$ if $u \in H^1(\mathbb{R}^3)$. Since $H^2(\mathbb{R}^3) \subset L^\infty(\mathbb{R}^3)$, we have

$$(7.9) \quad u \in H^2(\mathbb{R}^3) \implies |x|^{-1}u \in L^2(\mathbb{R}^3),$$

so

$$(7.10) \quad \mathcal{D}(H) \supset H^2(\mathbb{R}^3).$$

Indeed, we have:

Proposition 7.2. *For the self-adjoint extension H of $-\Delta - K|x|^{-1}$ defined above,*

$$(7.11) \quad \mathcal{D}(H) = H^2(\mathbb{R}^3).$$

Proof. Pick λ in the resolvent set of H ; for instance, $\lambda \in \mathbb{C} \setminus \mathbb{R}$. If $u \in \mathcal{D}(H)$ and $(H - \lambda)u = f \in L^2(\mathbb{R}^3)$, we have

$$(7.12) \quad u - KR_\lambda V u = R_\lambda f = g_\lambda,$$

where $V(x) = |x|^{-1}$ and $R_\lambda = (-\Delta - \lambda)^{-1}$. Now the operator of multiplication by $V(x) = |x|^{-1}$ has the property

$$(7.13) \quad M_V : H^1(\mathbb{R}^3) \longrightarrow L^{2-\varepsilon}(\mathbb{R}^3),$$

for all $\varepsilon > 0$, since $H^1(\mathbb{R}^3) \subset L^6(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ and $V \in L^{3-\varepsilon}$ on $|x| < 1$. Hence

$$M_V : H^1(\mathbb{R}^3) \longrightarrow H^{-\varepsilon}(\mathbb{R}^3),$$

for all $\varepsilon > 0$. Let us apply this to (7.12). We know that $u \in \mathcal{D}(H) \subset \mathcal{D}(H^{1/2}) = H^1(\mathbb{R}^3)$, so $KR_\lambda V u \in H^{2-\varepsilon}(\mathbb{R}^3)$. Thus $u \in H^{2-\varepsilon}(\mathbb{R}^3)$, for all $\varepsilon > 0$. But, for $\varepsilon > 0$ small enough,

$$(7.14) \quad M_V : H^{2-\varepsilon}(\mathbb{R}^3) \longrightarrow L^2(\mathbb{R}^3),$$

so then $u = KR_\lambda(Vu) + R_\lambda f \in H^2(\mathbb{R}^3)$. This proves that $\mathcal{D}(H) \subset H^2(\mathbb{R}^3)$ and gives (7.11).

Since H is self-adjoint, its spectrum is a subset of the real axis, $(-\infty, \infty)$. We next show that there is only point spectrum in $(-\infty, 0)$

Proposition 7.3. *The part of $\text{spec } H$ lying in $\mathbb{C} \setminus [0, \infty)$ is a bounded, discrete subset of $(-\infty, 0)$, consisting of eigenvalues of finite multiplicity and having at most $\{0\}$ as an accumulation point.*

Proof. Consider the equation $(H - \lambda)u = f \in L^2(\mathbb{R}^3)$, that is,

$$(7.15) \quad (-\Delta - \lambda)u - KVu = f,$$

with $V(x) = |x|^{-1}$ as before. Applying $R_\lambda = (-\Delta - \lambda)^{-1}$ to both sides, we again obtain (7.12):

$$(7.16) \quad (I - KR_\lambda M_V)u = g_\lambda = R_\lambda f.$$

Note that R_λ is a holomorphic function of $\lambda \in \mathbb{C} \setminus [0, \infty)$, with values in $\mathcal{L}(L^2(\mathbb{R}^3), H^2(\mathbb{R}^3))$. A key result in the analysis of (7.16) is the following:

Lemma 7.4. *For $\lambda \in \mathbb{C} \setminus [0, \infty)$,*

$$(7.17) \quad R_\lambda M_V \in \mathcal{K}(L^2(\mathbb{R}^3)),$$

where \mathcal{K} is the space of compact operators.

We will establish this via the following basic tool. For $\lambda \in \mathbb{C} \setminus [0, \infty)$, $\varphi \in C_0(\mathbb{R}^3)$, the space of continuous functions vanishing at infinity, we have

$$(7.18) \quad M_\varphi R_\lambda \in \mathcal{K}(L^2) \text{ and } R_\lambda M_\varphi \in \mathcal{K}(L^2).$$

To see this, note that, for $\varphi \in C_0^\infty(\mathbb{R}^3)$, the first inclusion in (7.18) follows from Rellich's theorem. Then this inclusion holds for uniform limits of such φ , hence for $\varphi \in C_0(\mathbb{R}^3)$. Taking adjoints yields the rest of (7.18).

Now, to establish (7.17), write

$$(7.19) \quad V = V_1 + V_2,$$

where $V_1 = \psi V$, $\psi \in C_0^\infty(\mathbb{R}^3)$, $\psi(x) = 1$ for $|x| \leq 1$. Then $V_2 \in C_0(\mathbb{R}^3)$, so $R_\lambda M_{V_2} \in \mathcal{K}$. We have $V_1 \in L^q(\mathbb{R}^3)$, for all $q \in [1, 3)$, so, taking $q = 2$, we have

$$(7.20) \quad M_{V_1} : L^2(\mathbb{R}^3) \longrightarrow L^1(\mathbb{R}^3) \subset H^{-3/2-\varepsilon}(\mathbb{R}^3),$$

for all $\varepsilon > 0$, hence

$$(7.21) \quad R_\lambda M_{V_1} : L^2(\mathbb{R}^3) \longrightarrow H^{1/2-\varepsilon}(\mathbb{R}^3) \subset L^2(\mathbb{R}^3).$$

Given V_1 supported on a ball B_R , the operator norm in (7.21) is bounded by a constant times $\|V_1\|_{L^2}$. You can approximate V_1 in L^2 -norm by a sequence $w_j \in C_0^\infty(\mathbb{R}^3)$. It follows that $R_\lambda M_{V_1}$ is a norm limit of a sequence of compact operators on $L^2(\mathbb{R}^3)$, so it is also compact, and (7.17) is established.

The proof of Proposition 7.4 is finished by the following result, which can be found as Proposition 7.4 in Chap. 9

Proposition 7.5. *Let \mathcal{O} be a connected, open set in \mathbb{C} . Suppose $C(\lambda)$ is a compact-operator-valued holomorphic function of $\lambda \in \mathcal{O}$. If $I - C(\lambda)$ is invertible at one point $p \in \mathcal{O}$, then it is invertible except at most on a discrete set in \mathcal{O} , and $(I - C(\lambda))^{-1}$ is meromorphic on \mathcal{O} .*

This applies to our situation, with $C(\lambda) = KR_\lambda M_V$; we know that $I - C(\lambda)$ is invertible for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$ in this case.

One approach to analyzing the negative eigenvalues of H is to use polar coordinates. If $-K|x|^{-1}$ is replaced by any radial potential $\mathcal{V}(|x|)$, the eigenvalue equation $Hu = -Eu$ becomes

$$(7.22) \quad \frac{\partial^2 u}{\partial r^2} + \frac{2}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \Delta_S u - \mathcal{V}(r)u = Eu.$$

We can use separation of variables, writing $u(r\theta) = v(r)\varphi(\theta)$, where φ is an eigenfunction of Δ_S , the Laplace operator on S^2 ,

$$(7.23) \quad \Delta_S \varphi = -\lambda \varphi, \quad \lambda = \left(k + \frac{1}{2}\right)^2 - \frac{1}{4} = k^2 + k.$$

Then we obtain for $v(r)$ the ODE

$$(7.24) \quad v''(r) + \frac{2}{r}v'(r) + f(r)v(r) = 0, \quad f(r) = -E - \frac{\lambda}{r^2} - \mathcal{V}(r).$$

One can eliminate the term involving v' by setting

$$(7.25) \quad w(r) = rv(r).$$

Then

$$(7.26) \quad w''(r) + f(r)w(r) = 0.$$

For the Coulomb problem, this becomes

$$(7.27) \quad w''(r) + \left[-E + \frac{K}{r} - \frac{\lambda}{r^2}\right]w(r) = 0.$$

If we set $W(r) = w(\beta r)$, $\beta = 1/2\sqrt{E}$, we get a form of Whittaker's ODE:

$$(7.28) \quad W''(z) + \left[-\frac{1}{4} + \frac{\kappa}{z} + \frac{\frac{1}{4} - \mu^2}{z^2}\right]W(z) = 0,$$

with

$$(7.29) \quad \kappa = \frac{K}{2\sqrt{E}}, \quad \mu^2 = \lambda + \frac{1}{4} = \left(k + \frac{1}{2}\right)^2.$$

This in turn can be converted to the confluent hypergeometric equation

$$(7.30) \quad z\psi''(z) + (b - z)\psi'(z) - a\psi(z) = 0$$

upon setting

$$(7.31) \quad W(z) = z^{\mu+1/2} e^{-z/2} \psi(z),$$

with

$$(7.32) \quad a = \mu - \kappa + \frac{1}{2} = k + 1 - \frac{K}{2\sqrt{E}},$$

$$b = 2\mu + 1 = 2k + 2.$$

Note that ψ and v are related by

$$(7.33) \quad v(r) = (2\sqrt{E})^{k+1} r^k e^{-2\sqrt{E}r} \psi(2\sqrt{E}r).$$

Looking at (7.28), we see that there are two independent solutions, one behaving roughly like $e^{-z/2}$ and the other like $e^{z/2}$, as $z \rightarrow +\infty$. Equivalently, (7.30) has two linearly independent solutions, a “good” one growing more slowly than exponentially and a “bad” one growing like e^z , as $z \rightarrow +\infty$. Of course, for a solution to give rise to an eigenfunction, we need $v \in L^2(\mathbb{R}^+, r^2 dr)$, that is, $w \in L^2(\mathbb{R}^+, dr)$. We need to have simultaneously $w(z) \sim ce^{-z/2}$ (roughly) as $z \rightarrow +\infty$ and w square integrable near $z = 0$. In view of (7.8), we also need $v' \in L^2(\mathbb{R}^+, r^2 dr)$.

To examine the behavior near $z = 0$, note that the Euler equation associated with (7.28) is

$$(7.34) \quad z^2 W''(z) + \left(\frac{1}{4} - \mu^2\right) W(z) = 0,$$

with solutions $z^{1/2+\mu}$ and $z^{1/2-\mu}$, i.e., z^{k+1} and z^{-k} , $k = 0, 1, 2, \dots$. If $k = 0$, both are square integrable near 0, but for $k \geq 1$ only one is. Going to the confluent hypergeometric equation (7.30), we see that two linearly independent solutions behave respectively like z^0 and $z^{-2\mu} = z^{-2k-1}$ as $z \rightarrow 0$.

As a further comment on the case $k = 0$, note that a solution W behaving like z^0 at $z = 0$ gives rise to $v(r) \sim C/r$ as $r \rightarrow 0$, with $c \neq 0$, hence $v'(r) \sim -C/r^2$. This is not square integrable near $r = 0$, with respect to $r^2 dr$, so also this case does not produce an eigenfunction of H .

If $b \notin \{0, -1, -2, \dots\}$, which certainly holds here, the solution to (7.30) that is “good” near $z = 0$ is given by the confluent hypergeometric function

$$(7.35) \quad {}_1F_1(a; b; z) = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} \frac{z^n}{n!},$$

an entire function of z . Here, $(a)_n = a(a+1)\cdots(a+n-1)$; $(a)_0 = 1$. If also $a \notin \{0, -1, -2, \dots\}$, it can be shown that

$$(7.36) \quad {}_1F_1(a; b; z) \sim \frac{\Gamma(b)}{\Gamma(a)} e^z z^{-(b-a)}, \quad z \rightarrow +\infty.$$

See the exercises below for a proof of this. Thus the “good” solution near $z = 0$ is “bad” as $z \rightarrow +\infty$, *unless* a is a nonpositive integer, say $a = -j$. In that case, as is clear from (7.35), ${}_1F_1(-j; b; z)$ is a polynomial in z , thus “good” as $z \rightarrow +\infty$. Thus the negative eigenvalues of H are given by $-E$, with

$$(7.37) \quad \frac{K}{2\sqrt{E}} = j + k + 1 = n,$$

that is, by

$$(7.38) \quad E = \frac{K^2}{4n^2}, \quad n = 1, 2, 3, \dots$$

Note that, for each value of n , one can write $n = j + k + 1$ using n choices of $k \in \{0, 1, 2, \dots, n-1\}$. For each such k , the $(k^2 + k)$ -eigenspace of Δ_S has dimension $2k + 1$, as established in Corollary 4.3. Thus the eigenvalue $-E = -K^2/4n^2$ of H has multiplicity

$$(7.39) \quad \sum_{k=0}^{n-1} (2k + 1) = n^2.$$

Let us denote by V_n the n^2 -dimensional eigenspace of H , associated to the eigenvalue $\lambda_n = -K^2/4n^2$.

The rotation group $\mathrm{SO}(3)$ acts on each V_n , via

$$\rho(g)f(x) = f(g^{-1}x), \quad g \in \mathrm{SO}(3), \quad x \in \mathbb{R}^3$$

By the analysis leading to (7.39), this action on V_n is not irreducible, but rather has n irreducible components. This suggests that there is an extra symmetry, and indeed, as W. Pauli discovered early in the history of quantum mechanics, there is one, arising via the Lenz vector (briefly introduced in §16 of Chap. 1), which we proceed to define.

The angular momentum vector $\mathbf{L} = \mathbf{x} \times \mathbf{p}$, with \mathbf{p} replaced by the vector operator $(\partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3)$, commutes with H as a consequence of the rotational invariance of H . The components of \mathbf{L} are

$$(7.40) \quad L_\ell = x_j \frac{\partial}{\partial x_k} - x_k \frac{\partial}{\partial x_j},$$

where (j, k, ℓ) is a cyclic permutation of $(1, 2, 3)$. Then the Lenz vector is defined by

$$(7.41) \quad \mathbf{B} = \frac{1}{K} (\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L}) - \frac{\mathbf{x}}{r},$$

with components B_j , $1 \leq j \leq 3$, each of which is a second-order differential operator, given explicitly by

$$(7.42) \quad B_j = \frac{1}{K} (L_k \partial_\ell + \partial_\ell L_k - L_\ell \partial_k - \partial_k L_\ell) - \frac{x_j}{r},$$

where (j, k, ℓ) is a cyclic permutation of $(1, 2, 3)$. A calculation gives

$$(7.43) \quad [H, B_j] = 0,$$

in the sense that these operators commute on $C^\infty(\mathbb{R}^3 \setminus 0)$.

It follows that if $u \in V_n$, then $B_j u$ is annihilated by $H - \lambda_n$, on $\mathbb{R}^3 \setminus 0$. Now, we have just gone through an argument designed to glean from all functions that are so annihilated, those that are actually eigenfunctions of H . In view of that, it is important to establish the next lemma

Lemma 7.6. *We have*

$$(7.44) \quad B_j : V_n \longrightarrow V_n.$$

Proof. Let $u \in V_n$. We know that $u \in \mathcal{D}(H) = H^2(\mathbb{R}^3)$. Also, from the analysis of the ODE (7.28), we know that $u(x)$ decays as $|x| \rightarrow \infty$, roughly like $e^{-|\lambda_n|^{1/2}|x|}$. It follows from (7.42) that $B_j u \in L^2(\mathbb{R}^3)$. It will be useful to obtain a bit more regularity, using $V_n \subset \mathcal{D}(H^2)$ together with the following.

Proposition 7.7. *If $u \in \mathcal{D}(H^2)$, then, for all $\varepsilon > 0$,*

$$(7.45) \quad u \in H^{5/2-\varepsilon}(\mathbb{R}^3).$$

Furthermore,

$$(7.46) \quad g \in \mathcal{S}(\mathbb{R}^3), \ g(0) = 0 \implies gu \in H^{7/2-\varepsilon}(\mathbb{R}^3).$$

Proof. We proceed along the lines of the proof of Proposition 7.2, using (7.12), i.e.,

$$(7.47) \quad u = KR_\lambda V u + R_\lambda f,$$

where $f = (H - \lambda)u$, with λ chosen in $\mathbb{C} \setminus \mathbb{R}$. We know that $f = (H - \lambda)u$ belongs to $\mathcal{D}(H)$, so $R_\lambda f \in H^4(\mathbb{R}^3)$. We know that $u \in H^2(\mathbb{R}^3)$. Parallel to (7.13), we can show that, for all $\varepsilon > 0$,

$$(7.48) \quad M_V : H^2(\mathbb{R}^3) \longrightarrow H^{1/2-\varepsilon}(\mathbb{R}^3),$$

so $KR_\lambda V u \in H^{5/2-\varepsilon}(\mathbb{R}^3)$. This gives (7.45).

Now, multiply (7.47) by g and write

$$(7.49) \quad gu = KR_\lambda g V u + K[M_g, R_\lambda] V u + g R_\lambda f.$$

This time we have

$$M_{gV} : H^2(\mathbb{R}^3) \longrightarrow H^{3/2-\varepsilon}(\mathbb{R}^3),$$

so $R_\lambda g V u \in H^{7/2-\varepsilon}(\mathbb{R}^3)$. Furthermore,

$$(7.50) \quad [M_g, R_\lambda] = R_\lambda [\Delta, M_g] R_\lambda : H^s(\mathbb{R}^3) \longrightarrow H^{s+3}(\mathbb{R}^3),$$

so $[M_g, R_\lambda] V u \in H^{7/2-\varepsilon}(\mathbb{R}^3)$. This establishes (7.46).

We can now finish the proof of Lemma 7.6. Note that the second-order derivatives in B_j have a coefficient vanishing at 0. Keep in mind the known exponential decay of $u \in V_n$. Also note that $M_{x_j/r} : H^2(\mathbb{R}^3) \rightarrow H^{3/2-\varepsilon}(\mathbb{R}^3)$. Therefore,

$$(7.51) \quad u \in V_n \implies B_j u \in H^{3/2-\varepsilon}(\mathbb{R}^3).$$

Consequently,

$$(7.52) \quad \Delta(B_j u) \in H^{-1/2-\varepsilon}(\mathbb{R}^3), \text{ and } V(B_j u) \in L^1(\mathbb{R}^3) + L^2(\mathbb{R}^3).$$

Thus $(H - \lambda_n)(B_j u)$, which we know vanishes on $\mathbb{R}^3 \setminus \{0\}$, must vanish completely, since (7.52) does not allow for a nonzero quantity supported on $\{0\}$. Using (7.8), we conclude that $B_j u \in \mathcal{D}(H)$, and the lemma is proved.

With Lemma 7.6 established, we can proceed to study the action of B_j and L_j on V_n . When (j, k, ℓ) is a cyclic permutation of $(1, 2, 3)$, we have

$$(7.53) \quad [L_j, L_k] = L_\ell,$$

and, after a computation,

$$(7.54) \quad [L_j, B_k] = B_\ell, \quad [B_j, B_k] = -\frac{4}{K} H L_\ell.$$

Of course, (7.52) is the statement that L_j span the Lie algebra $\mathfrak{so}(3)$ of $\mathrm{SO}(3)$. The identities (7.54), when L_j and B_j act on V_n , can be rewritten as

$$(7.55) \quad [L_j, A_k] = A_\ell, \quad [A_j, A_k] = A_\ell, \quad A_j = \frac{K}{2\sqrt{-\lambda_n}} B_j.$$

If we set

$$(7.56) \quad \mathbf{M} = \frac{1}{2}(\mathbf{L} + \mathbf{A}), \quad \mathbf{N} = \frac{1}{2}(\mathbf{L} - \mathbf{A}),$$

we get, for cyclic permutations (j, k, ℓ) of $(1, 2, 3)$,

$$(7.57) \quad [M_j, M_k] = M_\ell, \quad [N_j, N_k] = N_\ell, \quad [M_j, N_{j'}] = 0,$$

which is clearly the set of commutation relations for the Lie algebra $\mathfrak{so}(3) \oplus \mathfrak{so}(3)$. We next aim to show that this produces an irreducible representation of $\mathrm{SO}(4)$ on V_n , and to identify this representation. A priori, of course, one certainly has a representation of $\mathrm{SU}(2) \times \mathrm{SU}(2)$ on V_n .

We now examine the behavior on V_n of the Casimir operators $M^2 = M_1^2 + M_2^2 + M_3^2$ and N^2 . A calculation using the definitions gives $\mathbf{B} \cdot \mathbf{L} = 0$, hence $\mathbf{A} \cdot \mathbf{L} = 0$, so, on V_n ,

$$\begin{aligned}
 (7.58) \quad M^2 = N^2 &= \frac{1}{4}(A^2 + L^2) \\
 &= \frac{1}{4}\left(L^2 - \frac{K^2}{4\lambda_n}B^2\right).
 \end{aligned}$$

We also have the following key identity:

$$(7.59) \quad K^2(B^2 - I) = 4H(L^2 + I),$$

which follows from the definitions by a straightforward computation. If we compare (7.58) and (7.59) on V_n , where $H = \lambda_n$, we get

$$(7.60) \quad 4M^2 = 4N^2 = -\left(1 + \frac{K^2}{4\lambda_n}\right)I \quad \text{on } V_n.$$

Now the representation σ_n we get of $\text{SU}(2) \times \text{SU}(2)$ on V_n is a direct sum (possibly with only one summand) of representations $D_{j/2} \otimes D_{j/2}$, where $D_{j/2}$ is the standard irreducible representation of $\text{SU}(2)$ on \mathbb{C}^{j+1} , defined in §9 of Appendix B. The computation (7.60) implies that all the copies in this sum are isomorphic, that is, for some $j = j(n)$,

$$(7.61) \quad \sigma_n = \bigoplus_{\ell=1}^{\mu} D_{j(n)/2} \otimes D_{j(n)/2}.$$

A dimension count gives $\mu(j(n) + 1)^2 = n^2$. Note that on $D_{j/2} \otimes D_{j/2}$, we have $M^2 = N^2 = (j/2)(j/2 + 1)$. Thus (7.60) implies $j(j + 2) = -1 + K^2/4\lambda_n$, or

$$(7.62) \quad \lambda_n = -\frac{K^2}{4(j + 1)^2}, \quad j = j(n).$$

Comparing (7.38), we have $(j + 1)^2 = n^2$, that is,

$$(7.63) \quad j(n) = n - 1.$$

Since we know that $\dim V_n = n^2$, this implies that there is just one summand in (7.61), so

$$(7.64) \quad \sigma_n = D_{(n-1)/2} \otimes D_{(n-1)/2}.$$

This is an irreducible representation of $\text{SU}(2) \times \text{SU}(2)$, which is a double cover of $\text{SO}(4)$,

$$\kappa : \text{SU}(2) \times \text{SU}(2) \longrightarrow \text{SO}(4).$$

It is clear that σ_n is the identity operator on both elements in $\ker \kappa$, and so σ_n actually produces an irreducible representation of $\text{SO}(4)$.

Let ρ_n denote the restriction to V_n of the representation ρ of $\mathrm{SO}(3)$ on $L^3(\mathbb{R}^3)$, described above. If we regard this as a representation of $\mathrm{SU}(2)$, it is clear that ρ_n is the composition of σ_n with the diagonal map $\mathrm{SU}(2) \rightarrow \mathrm{SU}(2) \times \mathrm{SU}(2)$. Results established in §9 of Appendix B imply that such a tensor-product representation of $\mathrm{SU}(2)$ has the decomposition into irreducible representations:

$$(7.65) \quad \rho_n \approx \bigoplus_{k=0}^{n-1} D_k.$$

This is also precisely the description of ρ_n given by the analysis leading to (7.39).

There are a number of other group-theoretic perspectives on the quantum Coulomb problem, which can be found in [Eng] and [GS2]. See also [Ad] and [Cor], Vol. 2.

Exercises

1. For $H = -\Delta - K|x|^{-1}$ with domain given by (7.8), show that

$$(7.66) \quad \mathcal{D}(H) = \{u \in L^2(\mathbb{R}^3) : -\Delta u - K|x|^{-1}u \in L^2(\mathbb{R}^3)\},$$

where a priori, if $u \in L^2(\mathbb{R}^3)$, then $\Delta u \in H^{-2}(\mathbb{R}^3)$ and $|x|^{-1}u \in L^1(\mathbb{R}^3) + L^2(\mathbb{R}^3) \subset H^{-2}(\mathbb{R}^3)$.

(Hint: Parallel the proof of Proposition 7.2. If u belongs to the right side of (7.66), and if you pick $\lambda \in \mathbb{C} \setminus \mathbb{R}$, then, as in (7.12),

$$(7.67) \quad u - KR_\lambda V u = R_\lambda f \in H^2(\mathbb{R}^3).$$

Complement (7.13) with

$$(7.68) \quad \begin{aligned} M_V : L^2(\mathbb{R}^3) &\longrightarrow \bigcap_{\varepsilon > 0} H^{-3/2-\varepsilon}(\mathbb{R}^3), \\ M_V : \bigcap_{\varepsilon > 0} H^{1/2-\varepsilon}(\mathbb{R}^3) &\longrightarrow \bigcap_{\delta > 0} H^{-3/4-\delta}(\mathbb{R}^3). \end{aligned}$$

(Indeed, sharper results can be obtained.) Then deduce from (7.67) first that $u \in H^{1/2-\varepsilon}(\mathbb{R}^3)$ and then that $u \in H^{5/4-\delta}(\mathbb{R}^3) \subset H^1(\mathbb{R}^3)$.

2. As a variant of (7.4), show that, for $u \in H^1(\mathbb{R}^3)$,

$$(7.69) \quad \int |x|^{-2} |u(x)|^2 dx \leq 4 \int |\nabla u(x)|^2 dx.$$

Show that 4 is the best possible constant on the right. (Hint: Use the Mellin transform to show that the spectrum of $r d/dr - 1/2$ on $L^2(\mathbb{R}^+, r^{-1} dr)$ (which coincides with the spectrum of $r d/dr$ on $L^2(\mathbb{R}^+, dr)$) is $\{is - 1/2 : s \in \mathbb{R}\}$, hence

$$(7.70) \quad \int_0^\infty |u(r)|^2 dr \leq 4 \int_0^\infty |u'(r)|^2 r^2 dr.$$

This is sometimes called an “uncertainty principle” estimate. Why might that be? (Cf. [RS], Vol. 2, p. 169.)

3. Show that $H = -\Delta - K/|x|$ has no non-negative eigenvalues, i.e., only continuous spectrum in $[0, \infty)$. (*Hint*: Study the behavior as $r \rightarrow +\infty$ of solutions to the ODE (7.28), when $-E$ is replaced by $+E \in [0, \infty)$. Consult [Olv] for techniques. See also [RS], Vol. 4, for general results.)
4. Generalize the propositions of this section, with modifications as needed, to other classes of potentials $V(x)$, such as

$$V \in L^2 + \varepsilon L^\infty,$$

the set of functions V such that, for each $\varepsilon > 0$, one can write $V = V_1 + V_2$, $V_1 \in L^2$, $\|V_2\|_{L^\infty} \leq \varepsilon$. Consult [RS], Vols. 2–4, for further generalizations.

Exercises on the confluent hypergeometric function

1. Taking (7.35) as the definition of ${}_1F_1(a; b; z)$, show that

$$(7.71) \quad {}_1F_1(a; b; z) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)} \int_0^1 e^{zt} t^{a-1} (1-t)^{b-a-1} dt, \\ \text{Re } b > \text{Re } a > 0.$$

(*Hint*: Use the beta function identity, (A.23)–(A.24) of Chap. 3.) Show that (7.71) implies the asymptotic behavior (7.36), provided $\text{Re } b > \text{Re } a > 0$, but that this is insufficient for making the deduction (7.37).

Exercises 2–5 deal with the analytic continuation of (7.71) in a and b , and a complete justification of (7.36). To begin, write

$$(7.72) \quad {}_1F_1(a; b; z) = \frac{\Gamma(b)}{\Gamma(b-a)} A_\psi(a, -z) + \frac{\Gamma(b)}{\Gamma(a)} A_\varphi(b-a, z) e^z,$$

where, for $\text{Re } c > 0$, $\psi \in C^\infty([0, 1/2])$, we set

$$(7.73) \quad A_\psi(c, z) = \frac{1}{\Gamma(c)} \int_0^{1/2} e^{-zt} \psi(t) t^{c-1} dt,$$

and, in (7.72),

$$\psi(t) = (1-t)^{b-a-1}, \quad \varphi(t) = (1-t)^{a-1}.$$

2. Given $\text{Re } c > 0$, show that

$$(7.74) \quad A_\psi(c, z) \sim \psi(0) z^{-c}, \quad z \rightarrow +\infty,$$

and

$$(7.75) \quad A_\psi(c, -z) \sim \frac{\psi(\frac{1}{2})}{\Gamma(c)} z^{-1} e^{z/2}, \quad z \rightarrow +\infty.$$

3. For $j = 0, 1, 2, \dots$, set

$$(7.76) \quad A_j(c, t) = \frac{1}{\Gamma(c)} \int_0^{1/2} e^{-zt} t^j t^{c-1} dt,$$

so $A_j(c, z) = A_\psi(c, z)$, with $\psi(t) = t^j$. Show that

$$A_j(c, z) = \frac{\Gamma(c+j)}{\Gamma(c)} z^{-c-j} - \frac{1}{\Gamma(c)} \int_{1/2}^{\infty} e^{-zt} t^{c+j-1} dt,$$

for $\operatorname{Re} z > 0$. Deduce that $A_j(c, t)$ is an entire function of c , for $\operatorname{Re} z > 0$, and that

$$A_j(c, z) \sim \frac{\Gamma(c+j)}{\Gamma(c)} z^{-c-j}, \quad z \rightarrow +\infty,$$

if $c \notin \{0, -1, -2, \dots\}$.

4. Given $k = 1, 2, 3, \dots$, write

$$\psi(t) = a_0 + a_1 t + \dots + a_{k-1} t^{k-1} + \psi_k(t) t^k, \quad \psi_k \in C^\infty\left(\left[0, \frac{1}{2}\right]\right)$$

Thus

$$(7.77) \quad A_\psi(c, z) = \sum_{j=0}^{k-1} a_j A_j(c, z) + \frac{1}{\Gamma(c)} \int_0^{1/2} e^{-zt} \psi_k(t) t^{k+c-1} dt.$$

Deduce that $A_\psi(c, z)$ can be analytically continued to $\operatorname{Re} c > -k$ when $\operatorname{Re} z > 0$ and that (7.74) continues to hold if $c \notin \{0, -1, -2, \dots\}$, $a_0 \neq 0$.

5. Using $t^{c-1} = c^{-1}(d/dt)t^c$ and integrating by parts, show that

$$(7.78) \quad A_0(c, z) = z A_0(c+1, z) - \frac{1}{2^c \Gamma(c+1)} e^{-z/2},$$

for $\operatorname{Re} c > 0$, all $z \in \mathbb{C}$. Show that this provides an entire analytic continuation of $A_0(c, z)$ and that (7.74)–(7.75) hold, for $\psi(t) = 1$. Using

$$A_j(c, z) = \frac{\Gamma(c+j)}{\Gamma(c)} A_0(c+j, z)$$

and (7.77), verify (7.75) for all $\psi \in C^\infty([0, 1/2])$. (Also again verify (7.74)). Hence, verify the asymptotic expansion (7.36).

The approach given above to (7.36) is one the author learned from conversations with A. N. Varchenko. In Exercises 6–15 below, we introduce another solution to the confluent hypergeometric equation and follow a path to the expansion (7.36) similar to one described in [Leb] and in [Olv].

6. Show that a solution to the ODE (7.30) is also given by

$$z^{1-b} {}_1F_1(1+a-b; 2-b; z),$$

in addition to ${}_1F_1(a; b; z)$, defined by (7.35). Assume $b \neq 0, -1, -2, \dots$. Set

$$(7.79) \quad \begin{aligned} \Psi(a; b; z) &= \frac{\Gamma(1-b)}{\Gamma(1+a-b)} {}_1F_1(a; b; z) \\ &+ \frac{\Gamma(b-1)}{\Gamma(a)} z^{1-b} {}_1F_1(1+a-b; 2-b; z). \end{aligned}$$

Show that the Wronskian is given by

$$W({}_1F_1(a; b; z), \Psi(a; b; z)) = -\frac{\Gamma(b)}{\Gamma(a)} z^{-b} e^z.$$

7. Show that

$$(7.80) \quad {}_1F_1(a; b; z) = e^z {}_1F_1(b - a; b; -z), \quad b \notin \{0, -1, -2, \dots\}$$

(Hint: Use the integral in Exercise 1, and set $s = 1 - t$, for the case $\operatorname{Re} b > \operatorname{Re} a > 0$.)

8. Show that

$$(7.81) \quad \Psi(a; b; z) = \frac{1}{\Gamma(a)} \int_0^\infty e^{-zt} t^{a-1} (1+t)^{b-a-1} dt, \quad \operatorname{Re} a > 0, \operatorname{Re} z > 0.$$

(Hint: First show that the right side solves (7.30). Then check the behavior as $z \rightarrow 0$.)

9. Show that

$$(7.82) \quad \Psi(a; b; z) = z\Psi(a+1; b+1; z) + (1-a-b)\Psi(a+1; b; z).$$

(Hint: To get this when $\operatorname{Re} a > 0$, use the integral expression (7.81) for $\Psi(a+1; b+1; z)$, write $ze^{-zt} = -(d/dt)e^{-zt}$, and integrate by parts.)

10. Show that

$$(7.83) \quad \begin{aligned} {}_1F_1(a; b; z) &= \frac{\Gamma(b)}{\Gamma(b-a)} e^{\pm\pi ai} \Psi(a; b; z) \\ &+ \frac{\Gamma(b)}{\Gamma(a)} e^{\pm\pi(a-b)i} e^z \Psi(b-a; b; -z), \end{aligned}$$

where $-z = e^{\mp\pi i} z$, $b \neq 0, -1, -2, \dots$ (Hint: Make use of (7.80) as well as (7.79).)

11. Using the integral representation (7.81), show that under the hypotheses $\delta > 0$, $b \notin \{0, -1, -2, \dots\}$, and $\operatorname{Re} a > 0$, we have

$$(7.84) \quad \Psi(a; b; z) \sim z^{-\alpha}, \quad |z| \rightarrow \infty,$$

in the sector

$$(7.85) \quad |\operatorname{Arg} z| \leq \frac{\pi}{2} - \delta.$$

12. Extend (7.84) to the sector $|\operatorname{Arg} z| \leq \pi - \delta$. (Hint: Replace (7.81) by an integral along the ray $\gamma = \{e^{i\alpha}s : 0 \leq s < \infty\}$, given $|\alpha| < \pi/2$.)

13. Further extend (7.84) to the case where no restriction is placed on $\operatorname{Re} a$. (Hint: Use (7.82).)

14. Extend (7.84) still further, to be valid for

$$(7.86) \quad |\operatorname{Arg} z| \leq \frac{3\pi}{2} - \delta.$$

(Hint: See Theorem 2.2 on p. 235 of [Olv], and its application to this problem on p. 256 of [Olv].)

15. Use (7.83)–(7.86) to prove (7.36), that is,

$$(7.87) \quad {}_1F_1(a; b; z) \sim \frac{\Gamma(b)}{\Gamma(a)} e^z z^{-(b-a)}, \quad z \rightarrow +\infty,$$

provided $a, b \notin \{0, -1, -2, \dots\}$.

Remarks: For the analysis of $\Psi(b-a; b; -z)$ as $z \rightarrow +\infty$, the result of Exercise 14 suffices, but the result of Exercise 13 does not. This point appears to have been neglected in the discussion of (7.87) on p. 271 of [Leb].

8. The Laplace operator on cones

Generally, if N is any compact Riemannian manifold of dimension m , possibly with boundary, the cone over N , $C(N)$, is the space $\mathbb{R}^+ \times N$ together with the Riemannian metric

$$(8.1) \quad dr^2 + r^2 g,$$

where g is the metric tensor on N . In particular, a cone with vertex at the origin in \mathbb{R}^{m+1} can be described as the cone over a subdomain Ω of the unit sphere S^m in \mathbb{R}^{m+1} . Our purpose is to understand the behavior of the Laplace operator Δ , a negative, self-adjoint operator, on $C(N)$. If $\partial N \neq \emptyset$, we impose Dirichlet boundary conditions on $\partial C(N)$, though many other boundary conditions could be equally easily treated. The analysis here follows [CT].

The initial step is to use the method of separation of variables, writing Δ on $C(N)$ in the form

$$(8.2) \quad \Delta = \frac{\partial^2}{\partial r^2} + \frac{m}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \Delta_N,$$

where Δ_N is the Laplace operator on the base N . Let μ_j , $\varphi_j(x)$ denote the eigenvalues and eigenfunctions of $-\Delta_N$ (with Dirichlet boundary condition on ∂N if $\partial N \neq \emptyset$), and set

$$(8.3) \quad v_j = (\mu_j + \alpha^2)^{1/2}, \quad \alpha = -\frac{m-1}{2}.$$

If

$$g(r, x) = \sum_j g_j(r) \varphi_j(x),$$

with $g_j(r)$ well behaved, and if we define the second-order operator L_μ by

$$(8.4) \quad L_\mu g(r) = \left(\frac{\partial^2}{\partial r^2} + \frac{m}{r} \frac{\partial}{\partial r} - \frac{\mu}{r^2} \right) g(r),$$

then we have

$$(8.5) \quad \Delta g(r, x) = \sum_j L_{\mu_j} g_j(r) \varphi_j(x).$$

In particular,

$$(8.6) \quad \Delta(g_j \varphi_j) = -\lambda_j^2 g_j \varphi_j$$

provided

$$(8.7) \quad g_j(r) = r^{-(m-1)/2} J_{\nu_j}(\lambda r).$$

Here $J_\nu(z)$ is the Bessel function, introduced in §6 of Chap. 3; there in (6.6) it is defined to be

$$(8.8) \quad J_\nu(z) = \frac{(z/2)^\nu}{\Gamma(\frac{1}{2})\Gamma(\nu + \frac{1}{2})} \int_{-1}^1 (1-t^2)^{\nu-1/2} e^{izt} dt,$$

for $\operatorname{Re} \nu > -1/2$; in (6.11) we establish Bessel's equation

$$(8.9) \quad \left[\frac{d^2}{dz^2} + \frac{1}{z} \frac{d}{dz} + \left(1 - \frac{\nu^2}{z^2} \right) \right] J_\nu(z) = 0,$$

which justifies (8.6); and in (6.19) we produced the formula

$$(8.10) \quad J_\nu(z) = \left(\frac{z}{2} \right)^\nu \sum_{k=0}^{\infty} \frac{(-1)^k}{k! \Gamma(k + \nu + 1)} \left(\frac{z}{2} \right)^{2k}.$$

We also recall, from (6.56) of Chap. 3, the asymptotic behavior

$$(8.11) \quad J_\nu(r) \sim \left(\frac{2}{\pi r} \right)^{1/2} \cos\left(r - \frac{\pi \nu}{2} - \frac{\pi}{4}\right) + O(r^{-3/2}), \quad r \rightarrow +\infty.$$

This suggests making use of the Hankel transform, defined for $\nu \in \mathbb{R}^+$ by

$$(8.12) \quad H_\nu(g)(\lambda) = \int_0^\infty g(r) J_\nu(\lambda r) r dr.$$

Clearly, $H_\nu : C_0^\infty((0, \infty)) \rightarrow L^\infty(\mathbb{R}^+)$. We will establish the following:

Proposition 8.1. *For $\nu \geq 0$, H_ν extends uniquely from $C_0^\infty((0, \infty))$ to*

$$(8.13) \quad H_\nu : L^2(\mathbb{R}^+, r dr) \longrightarrow L^2(\mathbb{R}^+, \lambda d\lambda), \quad \text{unitary}.$$

Furthermore, for each $g \in L^2(\mathbb{R}^+, r dr)$,

$$(8.14) \quad H_\nu \circ H_\nu g = g.$$

To prove this, it is convenient to consider first

$$(8.15) \quad \widetilde{H}_\nu f(\lambda) = \int_0^\infty f(r) \frac{J_\nu(\lambda r)}{(\lambda r)^\nu} r^{2\nu+1} dr,$$

since, by (8.10), $(\lambda r)^{-\nu} J_\nu(\lambda r)$ is a smooth function of λr . Set

$$(8.16) \quad \mathcal{S}(\mathbb{R}^+) = \{f|_{\mathbb{R}^+} : f \in \mathcal{S}(\mathbb{R}) \text{ is even}\}.$$

Lemma 8.2. *If $\nu \geq -1/2$, then*

$$(8.17) \quad \widetilde{H}_\nu : \mathcal{S}(\mathbb{R}^+) \longrightarrow \mathcal{S}(\mathbb{R}^+).$$

Proof. By (8.10), $J_\nu(\lambda r)/(\lambda r)^\nu$ is a smooth function of λr . The formula (8.8) yields

$$(8.18) \quad \left| \frac{J_\nu(\lambda r)}{(\lambda r)^\nu} \right| \leq C_\nu < \infty,$$

for $\lambda r \in [0, \infty)$, $\nu > -1/2$, a result that, by the identity

$$(8.19) \quad J_{-1/2}(z) = \left(\frac{2}{\pi z} \right)^{1/2} \cos z,$$

established in (6.35) of Chap. 3, also holds for $\nu = -1/2$. This readily yields

$$(8.20) \quad \widetilde{H}_\nu : \mathcal{S}(\mathbb{R}^+) \longrightarrow L^\infty(\mathbb{R}^+),$$

whenever $\nu \geq -1/2$. Now consider the differential operator \widetilde{L}_ν , given by

$$(8.21) \quad \begin{aligned} \widetilde{L}_\nu f(r) &= -r^{-2\nu-1} \frac{\partial}{\partial r} \left(r^{2\nu+1} \frac{\partial f}{\partial r} \right) \\ &= -\frac{\partial^2 f}{\partial r^2} - \frac{2\nu+1}{r} \frac{\partial f}{\partial r}. \end{aligned}$$

Using Bessel's equation (8.9), we have

$$(8.22) \quad \widetilde{L}_\nu \left(\frac{J_\nu(\lambda r)}{(\lambda r)^\nu} \right) = \lambda^2 \frac{J_\nu(\lambda r)}{(\lambda r)^\nu},$$

and, for $f \in \mathcal{S}(\mathbb{R}^+)$,

$$(8.23) \quad \begin{aligned} \widetilde{H}_\nu(\widetilde{L}_\nu f)(\lambda) &= \lambda^2 \widetilde{H}_\nu f(\lambda), \\ \widetilde{H}_\nu(r^2 f)(\lambda) &= \widetilde{L}_\nu \widetilde{H}_\nu f(\lambda). \end{aligned}$$

Since $f \in L^\infty(\mathbb{R}^+)$ belongs to $\mathcal{S}(\mathbb{R}^+)$ if and only if arbitrary iterated applications of \widetilde{L}_ν and multiplication by r^2 to f yield elements of $L^\infty(\mathbb{R}^+)$, the result (8.17) follows. We also have that this map is continuous with respect to the natural Frechet space structure on $\mathcal{S}(\mathbb{R}^+)$.

Lemma 8.3. *Consider the elements $E_b \in \mathcal{S}(\mathbb{R}^+)$, given for $b > 0$ by*

$$(8.24) \quad E_b(r) = e^{-br^2}.$$

We have

$$(8.25) \quad \widetilde{H}_\nu E_{1/2}(\lambda) = E_{1/2}(\lambda),$$

and more generally

$$(8.26) \quad \widetilde{H}_\nu E_b(\lambda) = (2b)^{-\nu-1} E_{1/4b}(\lambda).$$

Proof. To establish (8.25), plug the power series (8.10) for $J_\nu(z)$ into (8.15) and integrate term by term, to get

$$(8.27) \quad \widetilde{H}_\nu E_{1/2}(\lambda) = \sum_{k=0}^{\infty} \frac{(-1)^k 2^{-\nu-2k}}{k! \Gamma(k + \nu + 1)} \lambda^{2k} \int_0^{\infty} r^{2k+2\nu+1} e^{-r^2/2} dr.$$

This last integral is seen to equal $2^{k+\nu} \Gamma(k + \nu + 1)$, so we have

$$(8.28) \quad \widetilde{H}_\nu E_{1/2}(\lambda) = \sum_{k=0}^{\infty} \frac{1}{k!} \left(-\frac{\lambda^2}{2} \right)^k = e^{-\lambda^2/2} = E_{1/2}(\lambda).$$

Having (8.25), we get (8.26) by an easy change of variable argument.

In more detail, set $r^2/2 = bs^2$, or $s = r/\sqrt{2b}$. Then set $\mu = \sqrt{2b}\lambda$, so $\lambda r = \mu s$. Then (8.28), which we can write as

$$(8.29) \quad \int_0^{\infty} e^{-r^2/2} J_\nu(\lambda r) r^{\nu+1} dr = \lambda^\nu e^{-\lambda^2/2},$$

translates to

$$(8.30) \quad \int_0^{\infty} e^{-bs^2} J_\nu(\mu s) (2b)^{(\nu+1)/2} s^{\nu+1} (2b)^{1/2} ds = (2b)^{-\nu/2} \mu^\nu e^{-\mu^2/4b},$$

or, changing notation back,

$$(8.31) \quad \int_0^{\infty} e^{-bs^2} J_\nu(\lambda s) s^{\nu+1} ds = (2b)^{-\nu-1} \lambda^\nu e^{-\lambda^2/4b},$$

which gives (8.26).

From (8.26) we have, for each $b > 0$,

$$(8.32) \quad \widetilde{H}_\nu \widetilde{H}_\nu E_b = (2b)^{-\nu-1} \widetilde{H}_\nu E_{1/4b} = E_b,$$

which verifies our stated Hankel inversion formula for $f = E_b$, $b > 0$. To get the inversion formula for general $f \in \mathcal{S}(\mathbb{R}^+)$, it suffices to establish the following.

Lemma 8.4. *The space*

$$(8.33) \quad \mathcal{V} = \text{Span}\{E_b : b > 0\}$$

is dense in $\mathcal{S}(\mathbb{R}^+)$.

Proof. Let $\overline{\mathcal{V}}$ denote the closure of \mathcal{V} in $\mathcal{S}(\mathbb{R}^+)$. From

$$(8.34) \quad \frac{1}{\varepsilon}(e^{-br^2} - e^{-(b+\varepsilon)r^2}) \rightarrow r^2 e^{-br^2},$$

we deduce that $r^2 e^{-br^2} \in \overline{\mathcal{V}}$, and inductively, we get

$$(8.35) \quad r^{2j} e^{-br^2} \in \overline{\mathcal{V}}, \quad \forall j \in \mathbb{Z}^+.$$

From here, one has

$$(8.36) \quad (\cos \xi r) e^{-r^2} \in \overline{\mathcal{V}}, \quad \forall \xi \in \mathbb{R}.$$

Now each even $\omega \in \mathcal{S}'(\mathbb{R})$ annihilating (8.36) for all $\xi \in \mathbb{R}$ has the property that $e^{-r^2} \omega$ has Fourier transform zero, which implies $\omega = 0$. The assertion (8.33) then follows by the Hahn-Banach theorem.

Putting the results of Lemmas 8.2–8.4 together, we have

Proposition 8.5. *Given $v \geq -1/2$, we have*

$$(8.37) \quad \widetilde{H}_v \widetilde{H}_v f = f,$$

for all $f \in \mathcal{S}(\mathbb{R}^+)$.

We promote this to

Proposition 8.6. *If $v \geq -1/2$, we have a unique extension of \widetilde{H}_v from $\mathcal{S}(\mathbb{R}^+)$ to*

$$(8.38) \quad \widetilde{H}_v : L^2(\mathbb{R}^+, r^{2v+1} dr) \longrightarrow L^2(\mathbb{R}^+, \lambda^{2v+1} d\lambda),$$

as a unitary operator, and (8.37) holds for all $f \in L^2(\mathbb{R}^+, r^{2v+1} dr)$.

Proof. Take $f, g \in \mathcal{S}(\mathbb{R}^+)$, and use the inner product

$$(8.39) \quad (f, g) = \int_0^\infty f(r) \overline{g(r)} r^{2v+1} dr.$$

Using Fubini's theorem and the fact that $J_v(\lambda r)/(\lambda r)^v$ is real valued and symmetric in (λ, r) , we get the first identity in

$$(8.40) \quad (\widetilde{H}_v f, \widetilde{H}_v g) = (\widetilde{H}_v \widetilde{H}_v f, g) = (f, g),$$

the second identity following by Proposition 8.5. From here, given that the linear space $\mathcal{S}(\mathbb{R}^+) \subset L^2(\mathbb{R}^+, r^{2\nu+1} dr)$ is dense, the assertions of Proposition 8.6 are apparent.

We return to the Hankel transform (8.12). Note that

$$(8.41) \quad H_\nu(r^\nu f)(\lambda) = \lambda^\nu \widetilde{H}_\nu f(\lambda),$$

and that $M_\nu f(r) = r^\nu f(r)$ has the property that

$$(8.42) \quad M_\nu : L^2(\mathbb{R}^+, r^{2\nu+1} dr) \longrightarrow L^2(\mathbb{R}^+, r dr) \text{ is unitary.}$$

Thus Proposition 8.6 yields Proposition 8.1.

Another proof is sketched in the exercises. An elaboration of Hankel's original proof is given on pp. 456–464 of [Wat].

In view of (8.23) and (8.41), we have

$$(8.43) \quad \begin{aligned} H_\nu(r^{-\alpha} L_\mu g) &= \int_0^\infty L_\mu(r^\alpha J_\nu(\lambda r)) g r^m dr \\ &= -\lambda^2 \int_0^\infty g r^\alpha J_\nu(\lambda r) r^m dr \\ &= -\lambda^2 H_\nu(r^{-\alpha} g). \end{aligned}$$

Now from (8.5)–(8.13), it follows that the map \mathcal{H} given by

$$(8.44) \quad \mathcal{H}g = \left(H_{\nu_0}(r^{-\alpha} g_0), H_{\nu_1}(r^{-\alpha} g_1), \dots \right)$$

provides an isometry of $L^2(C(N))$ onto $L^2(\mathbb{R}^+, \lambda d\lambda, \ell^2)$, such that Δ is carried into multiplication by $-\lambda^2$. Thus (8.44) provides a spectral representation of Δ . Consequently, for well-behaved functions f , we have

$$(8.45) \quad \begin{aligned} f(-\Delta)g(r, x) \\ = r^\alpha \sum_j \int_0^\infty f(\lambda^2) J_{\nu_j}(\lambda r) \lambda \int_0^\infty s^{1-\alpha} J_{\nu_j}(\lambda s) g_j(s) ds d\lambda \varphi_j(x). \end{aligned}$$

Now we can interpret (8.45) in the following fashion. Define the operator ν on N by

$$(8.46) \quad \nu = (-\Delta_N + \alpha^2)^{1/2}.$$

Thus $\nu \varphi_j = \nu_j \varphi_j$. Identifying operators with their distributional kernels, we can describe the kernel of $f(-\Delta)$ as a function on $\mathbb{R}^+ \times \mathbb{R}^+$ taking values in operators on N , by the formula

$$\begin{aligned}
 (8.47) \quad f(-\Delta) &= (r_1 r_2)^\alpha \int_0^\infty f(\lambda^2) J_\nu(\lambda r_1) J_\nu(\lambda r_2) \lambda \, d\lambda \\
 &= K(r_1, r_2, \nu),
 \end{aligned}$$

since the volume element on $C(N)$ is $r^m \, dr \, dS(x)$ if the m -dimensional area element of N is $dS(x)$.

At this point it is convenient to have in hand some calculations of Hankel transforms, including some examples of the form (8.47). We establish some here; many more can be found in [Wat]. Generalizing (8.31), we can compute $\int_0^\infty e^{-br^2} J_\nu(\lambda r) r^{\mu+1} \, dr$ in a similar fashion, replacing the integral in (8.27) by

$$(8.48) \quad \int_0^\infty r^{2k+\mu+\nu+1} e^{-br^2} \, dr = \frac{1}{2} b^{-k-\mu/2-\nu/2-1} \Gamma\left(\frac{\mu}{2} + \frac{\nu}{2} + k + 1\right).$$

We get

$$\begin{aligned}
 (8.49) \quad & \int_0^\infty e^{-br^2} J_\nu(\lambda r) r^{\mu+1} \, dr \\
 &= \lambda^\nu 2^{-\nu-1} b^{-\mu/2-\nu/2-1} \sum_{k=0}^\infty \frac{\Gamma(\frac{\mu}{2} + \frac{\nu}{2} + k + 1)}{k! \Gamma(k + \nu + 1)} \left(-\frac{\lambda^2}{4b}\right)^k.
 \end{aligned}$$

We can express the infinite series in terms of the confluent hypergeometric function, introduced in §7. A formula equivalent to (7.35) is

$$(8.50) \quad {}_1F_1(a; b; z) = \frac{\Gamma(b)}{\Gamma(a)} \sum_{k=0}^\infty \frac{\Gamma(a+k)}{\Gamma(b+k)} \frac{z^k}{k!},$$

since $(a)_k = a(a+1)\cdots(a+k-1) = \Gamma(a+k)/\Gamma(a)$. We obtain, for $\operatorname{Re} b > 0$, $\operatorname{Re}(\mu + \nu) > -2$,

$$\begin{aligned}
 (8.51) \quad & \int_0^\infty e^{-br^2} J_\nu(\lambda r) r^{\mu+1} \, dr \\
 &= \lambda^\nu 2^{-\nu-1} b^{-\mu/2-\nu/2-1} \frac{\Gamma(\frac{\mu}{2} + \frac{\nu}{2} + 1)}{\Gamma(\nu + 1)} {}_1F_1\left(\frac{\mu}{2} + \frac{\nu}{2} + 1; \nu + 1; -\frac{\lambda^2}{4b}\right).
 \end{aligned}$$

We can apply a similar attack when e^{-br^2} is replaced by e^{-br} , obtaining

$$\begin{aligned}
 (8.52) \quad & \int_0^\infty e^{-br} J_\nu(\lambda r) r^{\mu-1} \, dr \\
 &= \left(\frac{\lambda}{2}\right)^\nu b^{-\mu-\nu} \sum_{k=0}^\infty \frac{\Gamma(\mu + \nu + 2k)}{k! \Gamma(\nu + k + 1)} \left(-\frac{\lambda^2}{2b^2}\right)^k,
 \end{aligned}$$

at least provided $\operatorname{Re} b > |\lambda|$, $\nu \geq 0$, and $\mu + \nu > 0$; here we use

$$(8.53) \quad \int_0^\infty e^{-br} r^{2k+\mu+\nu-1} dr = b^{-2k-\mu-\nu} \Gamma(\mu + \nu + 2k).$$

The duplication formula for the gamma function (see (A.22) of Chap. 3) implies

$$(8.54) \quad \Gamma(2k + \mu + \nu) = \pi^{-1/2} 2^{2k+\mu+\nu-1} \Gamma\left(\frac{\mu}{2} + \frac{\nu}{2} + k\right) \Gamma\left(\frac{\mu}{2} + \frac{\nu}{2} + k + \frac{1}{2}\right),$$

so the right side of (8.52) can be rewritten as

$$(8.55) \quad \pi^{-1/2} \lambda^\nu 2^{\mu-1} b^{-\mu-\nu} \sum_{k=0}^{\infty} \frac{\Gamma(\frac{\mu}{2} + \frac{\nu}{2} + k) \Gamma(\frac{\mu}{2} + \frac{\nu}{2} + \frac{1}{2} + k)}{k! \Gamma(\nu + 1 + k)} \left(-\frac{\lambda^2}{b^2}\right)^k.$$

This infinite series can be expressed in terms of the hypergeometric function, defined by

$$(8.56) \quad {}_2F_1(a_1, a_2; b; z) = \sum_{k=0}^{\infty} \frac{(a_1)_k (a_2)_k}{(b)_k} \frac{z^k}{k!} \\ = \frac{\Gamma(b)}{\Gamma(a_1) \Gamma(a_2)} \sum_{k=0}^{\infty} \frac{\Gamma(a_1 + k) \Gamma(a_2 + k)}{\Gamma(b + k)} \frac{z^k}{k!},$$

for $a_1, a_2 \notin \{0, -1, -2, \dots\}$, $|z| < 1$. If we put the sum in (8.55) into this form, and use the duplication formula, to write

$$\Gamma(a_1) \Gamma(a_2) = \Gamma\left(\frac{\mu}{2} + \frac{\nu}{2}\right) \Gamma\left(\frac{\mu}{2} + \frac{\nu}{2} + \frac{1}{2}\right) = \pi^{1/2} 2^{-\mu-\nu+1} \Gamma(\mu + \nu),$$

we obtain

$$(8.57) \quad \int_0^\infty e^{-br} J_\nu(\lambda r) r^{\mu-1} dr \\ = \left(\frac{\lambda}{2}\right)^\nu b^{-\mu-\nu} \frac{\Gamma(\mu + \nu)}{\Gamma(\nu + 1)} \cdot {}_2F_1\left(\frac{\mu}{2} + \frac{\nu}{2}, \frac{\mu}{2} + \frac{\nu}{2} + \frac{1}{2}; \nu + 1; -\frac{\lambda^2}{b^2}\right).$$

This identity, established so far for $|\lambda| < \operatorname{Re} b$ (and $\nu \geq 0$, $\mu + \nu > 0$), continues analytically to λ in a complex neighborhood of $(0, \infty)$.

To evaluate the integral (8.47) with $f(\lambda^2) = e^{-t\lambda^2}$, we can use the power series (8.10) for $J_\nu(\lambda r_1)$ and for $J_\nu(\lambda r_2)$ and integrate the resulting double series term by term using (8.48). We get

$$(8.58) \quad \int_0^\infty e^{-t\lambda^2} J_\nu(r_1 \lambda) J_\nu(r_2 \lambda) \lambda d\lambda \\ = \frac{1}{2t} \left(\frac{r_1 r_2}{4t}\right)^\nu \times \sum_{j,k \geq 0} \frac{\Gamma(\nu + j + k + 1)}{\Gamma(\nu + j + 1) \Gamma(\nu + k + 1)} \frac{1}{j! k!} \left(-\frac{r_1^2}{4t}\right)^j \left(-\frac{r_2^2}{4t}\right)^k,$$

for any $t, r_1, r_2 > 0$, $\nu \geq 0$. This can be written in terms of the modified Bessel function $I_\nu(z)$, given by

$$(8.59) \quad I_\nu(z) = \left(\frac{z}{2}\right)^\nu \sum_{k=0}^{\infty} \frac{1}{k! \Gamma(\nu + k + 1)} \left(\frac{z}{2}\right)^{2k}.$$

One obtains the following, known as the Weber identity.

Proposition 8.7. *For $t, r_1, r_2 > 0$,*

$$(8.60) \quad \int_0^\infty e^{-t\lambda^2} J_\nu(r_1\lambda) J_\nu(r_2\lambda) \lambda \, d\lambda = \frac{1}{2t} e^{-(r_1^2 + r_2^2)/4t} I_\nu\left(\frac{r_1 r_2}{2t}\right).$$

Proof. The left side of (8.60) is given by (8.58). Meanwhile, by (8.59), the right side of (8.60) is equal to $(1/2t)(r_1 r_2/4t)^\nu$ times

$$(8.61) \quad \sum_{\ell, m \geq 0} \frac{1}{\ell! m!} \left(-\frac{r_1^2}{4t}\right)^\ell \left(-\frac{r_2^2}{4t}\right)^m \sum_{n=0}^{\infty} \frac{1}{n! \Gamma(\nu + n + 1)} \left(\frac{r_1 r_2}{4t}\right)^{2n}.$$

If we set $y_j = -r_j^2/4t$, we see that the asserted identity (8.60) is equivalent to the identity

$$(8.62) \quad \begin{aligned} & \sum_{j, k \geq 0} \frac{\Gamma(\nu + j + k + 1)}{\Gamma(\nu + j + 1) \Gamma(\nu + k + 1)} \frac{1}{j! k!} y_1^j y_2^k \\ &= \sum_{\ell, m, n \geq 0} \frac{1}{\ell! m!} \frac{1}{n! \Gamma(\nu + n + 1)} y_1^{\ell+n} y_2^{m+n}. \end{aligned}$$

We compare coefficients of $y_1^j y_2^k$ in (8.62). Since both sides of (8.62) are symmetric in (y_1, y_2) , it suffices to treat the case

$$(8.63) \quad j \leq k,$$

which we assume henceforth. Then we take $\ell + n = j$, $m + n = k$ and sum over $n \in \{0, \dots, j\}$, to see that (8.62) is equivalent to the validity of

$$(8.64) \quad \sum_{n=0}^j \frac{1}{(j-n)!(k-n)!n! \Gamma(\nu + n + 1)} = \frac{\Gamma(\nu + j + k + 1)}{\Gamma(\nu + j + 1) \Gamma(\nu + k + 1)} \frac{1}{j! k!},$$

whenever $0 \leq j \leq k$. Using the identity

$$\Gamma(\nu + j + 1) = (\nu + j) \cdots (\nu + n + 1) \Gamma(\nu + n + 1)$$

and its analogues for the other Γ -factors in (8.64), we see that (8.64) is equivalent to the validity of

$$(8.65) \quad \sum_{n=0}^j \frac{j!k!}{(j-n)!(k-n)!n!} (v+j) \cdots (v+n+1) = (v+j+k) \cdots (v+k+1),$$

for $0 \leq j \leq k$. Note that the right side of (8.65) is a polynomial of degree j in v , and the general term on the left side of (8.65) is a polynomial of degree $j-n$ in v .

In order to establish (8.65), it is convenient to set

$$(8.66) \quad \mu = v + j$$

and consider the associated polynomial identity in μ . With

$$(8.67) \quad \begin{aligned} p_0(\mu) &= 1, & p_1(\mu) &= \mu, & p_2(\mu) &= \mu(\mu-1), \dots \\ p_j(\mu) &= \mu(\mu-1) \cdots (\mu-j+1), \end{aligned}$$

we see that $\{p_0, p_1, \dots, p_j\}$ is a basis of the space \mathcal{P}_j of polynomials of degree j in μ , and our task is to write

$$(8.68) \quad p_j(\mu+k) = (\mu+k)(\mu+k-1) \cdots (\mu+k-j+1)$$

as a linear combination of p_0, \dots, p_j . To this end, define

$$(8.69) \quad T : \mathcal{P}_j \longrightarrow \mathcal{P}_j, \quad Tp(\mu) = p(\mu+1).$$

By explicit calculation,

$$(8.70) \quad \begin{aligned} p_1(\mu+1) &= p_1(\mu) + p_0(\mu), \\ p_2(\mu+1) &= (\mu+1)\mu = \mu(\mu-1) + 2\mu = p_2(\mu) + 2p_1(\mu), \end{aligned}$$

and an inductive argument gives

$$(8.71) \quad Tp_i = p_i + ip_{i-1}.$$

By convention we set $p_i = 0$ for $i < 0$. Our goal is to compute $T^k p_j$. Note that

$$(8.72) \quad T = I + N, \quad Np_i = ip_{i-1},$$

and

$$(8.73) \quad T^k = \sum_{n=0}^k \binom{k}{n} N^n,$$

if $j \leq k$. By (8.72),

$$(8.74) \quad N^n p_i = i(i-1) \cdots (i-n+1) p_{i-n},$$

so we have

$$(8.75) \quad \begin{aligned} T^k p_j &= \sum_{n=0}^j \binom{k}{n} j(j-1) \cdots (j-n+1) p_{j-n} \\ &= \sum_{n=0}^j \frac{k!}{(k-n)!n!} \frac{j!}{(j-n)!} p_{j-n}. \end{aligned}$$

This verifies (8.65) and completes the proof of (8.60).

Similarly we can evaluate (8.47) with $f(\lambda^2) = e^{-t\lambda}/\lambda$, as an infinite series, using (8.53) to integrate each term of the double series. We get

$$(8.76) \quad \begin{aligned} &\int_0^\infty e^{-t\lambda} J_\nu(r_1\lambda) J_\nu(r_2\lambda) d\lambda \\ &= \frac{1}{t} \left(\frac{r_1 r_2}{t^2} \right)^\nu \sum_{j,k \geq 0} \frac{\Gamma(2\nu + 2j + 2k + 1)}{\Gamma(\nu + j + 1) \Gamma(\nu + k + 1)} \frac{1}{j!k!} \left(-\frac{r_1^2}{4t^2} \right)^j \left(-\frac{r_2^2}{4t^2} \right)^k, \end{aligned}$$

provided $t > r_j > 0$. It is possible to express this integral in terms of the Legendre function $Q_{\nu-1/2}(z)$.

Proposition 8.8. *One has, for all $y, r_1, r_2 > 0$, $\nu \geq 0$,*

$$(8.77) \quad \int_0^\infty e^{-y\lambda} J_\nu(r_1\lambda) J_\nu(r_2\lambda) d\lambda = \frac{1}{\pi} (r_1 r_2)^{-1/2} Q_{\nu-1/2} \left(\frac{r_1^2 + r_2^2 + y^2}{2r_1 r_2} \right).$$

The Legendre functions $P_{\nu-1/2}(z)$ and $Q_{\nu-1/2}(z)$ are solutions to

$$(8.78) \quad \frac{d}{dz} \left[(1-z^2) \frac{d}{dz} u(z) \right] + \left(\nu^2 - \frac{1}{4} \right) u(z) = 0;$$

Compare with (4.52). Extending (4.41), we can set

$$(8.79) \quad P_{\nu-1/2}(\cos \theta) = \frac{2}{\pi} \int_0^\theta (2 \cos s - 2 \cos \theta)^{-1/2} \cos \nu s \, ds,$$

and $Q_{\nu-1/2}(z)$ can be defined by the integral formula

$$(8.80) \quad Q_{\nu-1/2}(\cosh \eta) = \int_\eta^\infty (2 \cosh s - 2 \cosh \eta)^{-1/2} e^{-s\nu} \, ds.$$

The identity (8.77) is known as the *Lipschitz-Hankel integral formula*.

Proof of Proposition 8.8. We derive (8.77) from the Weber identity (8.60). Recall

$$(8.81) \quad I_\nu(y) = e^{-\pi i \nu/2} J_\nu(iy), \quad y > 0.$$

To work with (8.60), we use the subordination identity

$$(8.82) \quad e^{-y\lambda} = \frac{\lambda}{\sqrt{\pi}} \int_0^\infty e^{-y^2/4t} e^{-t\lambda^2} t^{-1/2} dt;$$

cf. Chap. 3, (5.31) for a proof. Plugging this into the left side of (8.77), and using (8.60), we see that the left side of (8.77) is equal to

$$(8.83) \quad \frac{1}{2\sqrt{\pi}} \int_0^\infty e^{-(r_1^2+r_2^2+y^2)/4t} I_\nu\left(\frac{r_1 r_2}{2t}\right) t^{-3/2} dt.$$

The change of variable $s = r_1 r_2 / 2t$ gives

$$(8.84) \quad \sqrt{\frac{1}{2\pi}} (r_1 r_2)^{-1/2} \int_0^\infty e^{-s(r_1^2+r_2^2+y^2)/2r_1 r_2} I_\nu(s) s^{-1/2} ds.$$

Thus the asserted identity (8.77) follows from the identity

$$(8.85) \quad \int_0^\infty e^{-sz} I_\nu(s) s^{-1/2} ds = \sqrt{\frac{2}{\pi}} Q_{\nu-1/2}(z), \quad z > 0.$$

As for the validity of (8.85), we mention two identities. Recall from (8.57) that

$$(8.86) \quad \int_0^\infty e^{-sz} J_\nu(\lambda s) s^{\mu-1} ds = \left(\frac{\lambda}{2}\right)^\nu z^{-\mu-\nu} \frac{\Gamma(\mu+\nu)}{\Gamma(\nu+1)} \cdot {}_2F_1\left(\frac{\mu}{2} + \frac{\nu}{2} + \frac{1}{2}, \frac{\mu}{2} + \frac{\nu}{2}; \nu+1; -\frac{\lambda^2}{z^2}\right).$$

Next, there is the classical representation of the Legendre function $Q_{\nu-1/2}(z)$ as a hypergeometric function:

$$(8.87) \quad Q_{\nu-1/2}(z) = \frac{\Gamma(\frac{1}{2}) \Gamma(\nu + \frac{1}{2})}{\Gamma(\nu+1)} (2z)^{-\nu-1/2} {}_2F_1\left(\frac{\nu}{2} + \frac{3}{4}, \frac{\nu}{2} + \frac{1}{4}; \nu+1; \frac{1}{z^2}\right);$$

cf. [Leb], (7.3.7) If we apply (8.86) with $\lambda = i$, $\mu = 1/2$ (keeping (8.81) in mind), then (8.85) follows.

Remark: Formulas (8.77) and (8.60) are proven in the opposite order in [W].

By analytic continuation, we can treat $f(\lambda^2) = e^{-\varepsilon\lambda}\lambda^{-1}\sin\lambda t$ for any $\varepsilon > 0$. We apply this to (8.47). Letting $\varepsilon \searrow 0$, we get for the fundamental solution to the wave equation:

$$\begin{aligned}
 & (-\Delta)^{-1/2} \sin t (-\Delta)^{1/2} \\
 (8.88) \quad &= -\lim_{\varepsilon \searrow 0} (r_1 r_2)^\alpha \operatorname{Im} \int_0^\infty e^{-(\varepsilon+it)\lambda} J_\nu(\lambda r_1) J_\nu(\lambda r_2) d\lambda \\
 &= -\frac{1}{\pi} (r_1 r_2)^{\alpha-1/2} \lim_{\varepsilon \searrow 0} \operatorname{Im} Q_{\nu-1/2} \left(\frac{r_1^2 + r_2^2 + (\varepsilon + it)^2}{2r_1 r_2} \right).
 \end{aligned}$$

Using the integral formula (8.80), where the path of integration is a suitable path from η to $+\infty$ in the complex plane, one obtains the following alternative integral representation of $(-\Delta)^{-1/2} \sin t (-\Delta)^{1/2}$. The Schwartz kernel is equal to

$$(8.89) \quad 0, \quad \text{if } t < |r_1 - r_2|,$$

$$(8.90) \quad \frac{1}{\pi} (r_1 r_2)^\alpha \int_0^{\beta_1} [t^2 - (r_1^2 + r_2^2 - 2r_1 r_2 \cos s)]^{-1/2} \cos \nu s \, ds,$$

if $|r_1 - r_2| < t < r_1 + r_2$, and

$$(8.91) \quad \frac{1}{\pi} (r_1 r_2)^\alpha \cos \pi \nu \int_{\beta_2}^\infty [r_1^2 + r_2^2 + 2r_1 r_2 \cosh s - t^2]^{-1/2} e^{-s\nu} \, ds,$$

if $t > r_1 + r_2$, where

$$(8.92) \quad \beta_1 = \cos^{-1} \left(\frac{r_1^2 + r_2^2 - t^2}{2r_1 r_2} \right), \quad \beta_2 = \cosh^{-1} \left(\frac{t^2 - r_1^2 - r_2^2}{2r_1 r_2} \right).$$

Recall that $\alpha = -(m-1)/2$, where $m = \dim N$.

We next show how formulas (8.89)–(8.91) lead to an analysis of the classical problem of diffraction of waves by a slit along the positive x -axis in the plane \mathbb{R}^2 . In fact, if waves propagate in \mathbb{R}^2 with this ray removed, on which Dirichlet boundary conditions are placed, we can regard the space as the cone over an interval of length 2π , with Dirichlet boundary conditions at the endpoints. By the method of images, it suffices to analyze the case of the cone over a circle of circumference 4π (twice the circumference of the standard unit circle). Thus $C(N)$ is a double cover of $\mathbb{R}^2 \setminus 0$ in this case. We divide up the spacetime into regions I, II, and III, respectively, as described by (8.89), (8.90), and (8.91). Region I contains only points on $C(N)$ too far away from the source point to be influenced by time t ; that the fundamental solution is 0 here is consistent with finite propagation speed.

Since the circle has dimension $m = 1$, we see that

$$(8.93) \quad \nu = (-\Delta_N)^{1/2} = \left(-\frac{d^2}{d\theta^2} \right)^{1/2}$$

in this case if $\theta \in \mathbb{R}/(4\pi\mathbb{Z})$ is the parameter on the circle of circumference 4π . On the line, we have

$$(8.94) \quad \cos s\nu \delta_{\theta_1}(\theta_2) = \frac{1}{2}[\delta(\theta_1 - \theta_2 + s) + \delta(\theta_1 - \theta_2 - s)].$$

To get $\cos s\nu$ on $\mathbb{R}/(4\pi\mathbb{Z})$, we simply make (8.94) periodic by the method of images. Consequently, from (8.90), the wave kernel $(-\Delta)^{-1/2} \sin t(-\Delta)^{1/2}$ is equal to

$$(8.95) \quad \begin{aligned} (2\pi)^{-1} [t^2 - r_1^2 - r_2^2 + 2r_1r_2 \cos(\theta_1 - \theta_2)]^{-1/2} & \quad \text{if } |\theta_1 - \theta_2| \leq \pi, \\ 0 & \quad \text{if } |\theta_1 - \theta_2| > \pi, \end{aligned}$$

in region II. Of course, for $|\theta_1 - \theta_2| < \pi$ this coincides with the free space fundamental solution, so (8.95) also follows by finite propagation speed.

We turn now to an analysis of region III. In order to make this analysis, it is convenient to make simultaneous use both of (8.91) and of another formula for the wave kernel in this region, obtained by choosing another path from η to ∞ in the integral representation (8.80). The formula (8.91) is obtained by taking a horizontal line segment; see Fig. 8.1.

If instead we take the path indicated in Fig. 8.2, we obtain the following formula for $(-\Delta)^{-1/2} \sin t(-\Delta)^{1/2}$ in region III:

$$(8.96) \quad \begin{aligned} \pi^{-1} (r_1 r_2)^{-(m-1)/2} & \left\{ \int_0^\pi (t^2 - r_1^2 - r_2^2 + 2r_1r_2 \cos s)^{-1/2} \cos s\nu \, ds \right. \\ & \left. - \sin \pi \nu \int_0^{\beta_2} (t^2 - r_1^2 - r_2^2 - 2r_1r_2 \cosh s)^{-1/2} e^{-s\nu} \, ds \right\}. \end{aligned}$$

The operator ν on $\mathbb{R}/(4\pi\mathbb{Z})$ given by (8.93) has spectrum consisting of

$$(8.97) \quad \text{Spec } \nu = \left\{ 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots \right\},$$

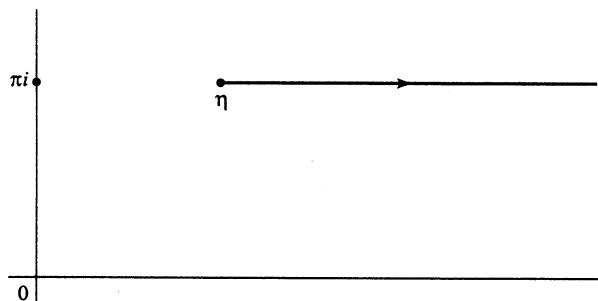


FIGURE 8.1 Integration Contour

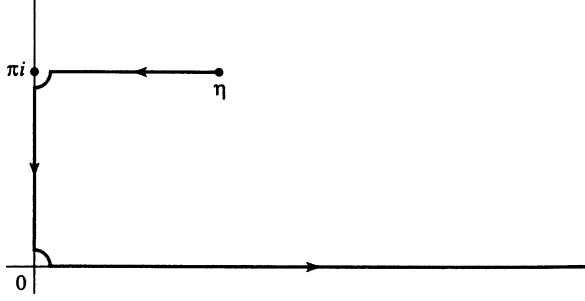


FIGURE 8.2 Alternative Contour

all the eigenvalues except for 0 occurring with multiplicity 2. The formula (8.91) shows the contribution coming from the half-integers in $\text{Spec } \nu$ vanishes, since $\cos \frac{1}{2}\pi n = 0$ if n is an odd integer. Thus we can use formula (8.96) and compose with the projection onto the sum of the eigenspaces of ν with integer spectrum. This projection is given by

$$(8.98) \quad P = \cos^2 \pi \nu$$

on $\mathbb{R}/(4\pi\mathbb{Z})$. Since $\sin \pi n = 0$, in the case $N = \mathbb{R}/(4\pi\mathbb{Z})$ we can rewrite (8.96) as

$$(8.99) \quad \pi^{-1}(r_1 r_2)^{-(m-1)/2} \int_0^\pi (t^2 - r_1^2 - r_2^2 + 2r_1 r_2 \cos s)^{-1/2} P \cos s \nu \, ds.$$

In view of the formulas (8.94) and (8.96), we have

$$(8.100) \quad \begin{aligned} & P \cos s \nu \delta_{\theta_1}(\theta_2) \\ &= \frac{1}{4} [\delta(\theta_1 - \theta_2 + s) + \delta(\theta_1 - \theta_2 - s) \\ &\quad + \delta(\theta_1 - \theta_2 + 2\pi + s) + \delta(\theta_1 - \theta_2 + 2\pi - s)] \mod 4\pi. \end{aligned}$$

Thus, in region III, we have for the wave kernel $(-\Delta)^{-1/2} \sin t(-\Delta)^{1/2}$ the formula

$$(8.101) \quad (4\pi)^{-1} (t^2 - r_1^2 - r_2^2 + 2r_1 r_2 \cos(\theta_1 - \theta_2))^{-1/2}.$$

Thus, in region III, the value of the wave kernel at points $(r_1, \theta_1), (r_2, \theta_2)$ of the double cover of $\mathbb{R}^2 \setminus 0$ is given by half the value of the wave kernel on \mathbb{R}^2 at the image points. The jump in behavior from (8.95) to (8.101) gives rise to a diffracted wave.

We depict the singularities of the fundamental solution to the wave equation for \mathbb{R}^2 minus a slit in Figs. 8.3 and 8.4. In Fig. 8.3 we have the situation $|t| < r_1$,

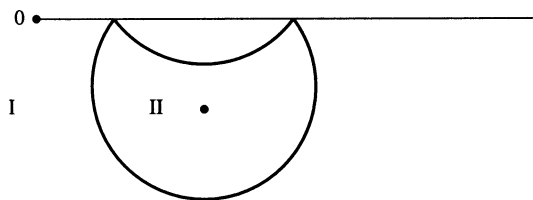


FIGURE 8.3 Reflected Wave Front

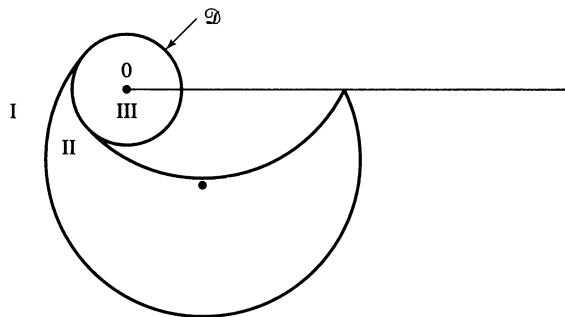


FIGURE 8.4 Reflected and Diffracted Wave Fronts

where no diffraction has occurred, and region III is empty. In Fig. 8.4 we have a typical situation for $|t| > r_1$, with the diffracted wave labeled by a “D.”

This diffraction problem was first treated by Sommerfeld [Som] and was the first diffraction problem to be rigorously analyzed. For other approaches to the diffraction problem presented above, see [BSU] and [Stk].

Generally, the solution (8.89)–(8.91) contains a diffracted wave on the boundary between regions II and III. In Fig. 8.5 we illustrate the diffraction of a wave by a wedge; here N is an interval of length $\ell < 2\pi$. We now want to provide, for general N , a description of the behavior of the distribution $v = (-\Delta)^{-1/2} \sin t (-\Delta)^{1/2} \delta_{(r_2, x_2)}$ near this diffracted wave, that is, a study of the limiting behavior as $r_1 \searrow t - r_2$ and as $r_1 \nearrow t - r_2$.

We begin with region II. From (8.90), we have v equal to

$$(8.102) \quad \frac{1}{2} (r_1 r_2)^{\alpha-1/2} P_{\nu-1/2}(\cos \beta_1) \delta_{x_2} \quad \text{in region II,}$$

where $P_{\nu-1/2}$ is the Legendre function defined by (8.79) and β_1 is given by (8.92). Note that as $r_1 \searrow t - r_2$, $\beta_1 \nearrow \pi$.

To analyze (8.102), replace s by $\pi - s$ in (8.79), and, with $\delta_1 = \pi - \beta_1$, write

$$(8.103) \quad \begin{aligned} \frac{\pi}{2} P_{\nu-1/2}(\cos \beta_1) &= \cos \pi \nu \int_{\delta_1}^{\pi} (2 \cos \delta_1 - 2 \cos s)^{-1/2} \cos s \nu \, ds \\ &\quad + \sin \pi \nu \int_{\delta_1}^{\pi} (2 \cos \delta_1 - 2 \cos s)^{-1/2} \sin s \nu \, ds. \end{aligned}$$

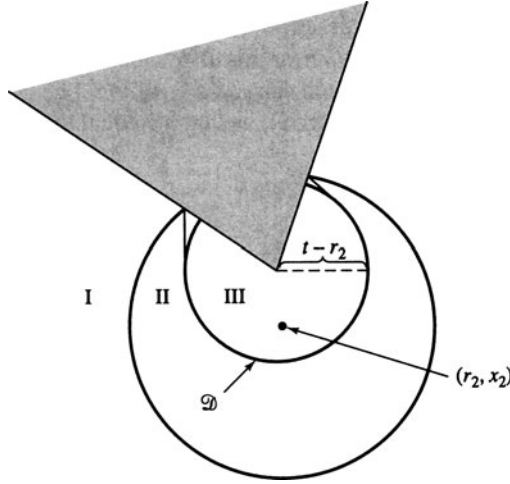


FIGURE 8.5 Diffraction by a Wedge

As $\delta_1 \searrow 0$, the second term on the right tends in the limit to

$$(8.104) \quad \sin \pi \nu \int_0^\pi \frac{\sin s \nu}{\sin \frac{1}{2}s} ds.$$

Write the first term on the right side of (8.103) as

$$(8.105) \quad \begin{aligned} & \cos \pi \nu \int_{\delta_1}^\pi (2 \cos \delta_1 - 2 \cos s)^{-1/2} (\cos s \nu - 1) ds \\ & + \cos \pi \nu \int_{\delta_1}^\pi (2 \cos \delta_1 - 2 \cos s)^{-1/2} ds. \end{aligned}$$

As $\delta_1 \searrow 0$, the first term here tends in the limit to

$$(8.106) \quad \cos \pi \nu \int_0^\pi \frac{\cos s \nu - 1}{\sin \frac{1}{2}s} ds.$$

The second integral in (8.105) is a scalar, independent of ν , and it is easily seen to have a logarithmic singularity. More precisely,

$$(8.107) \quad \begin{aligned} & \int_{\delta_1}^\pi (2 \cos \delta_1 - 2 \cos s)^{-\frac{1}{2}} ds \\ & \sim \left(\log \frac{2}{\delta_1} \right) \sum_{j=0}^\infty A_j \delta_1^j + \sum_{j=1}^\infty B_j \delta_1^j, \quad A_0 = 1. \end{aligned}$$

Consequently, one derives the following.

Proposition 8.9. Fix (r_2, x_2) and t . Then, as $r_1 \searrow t - r_2$,

$$(8.108) \quad \begin{aligned} & (-\Delta)^{-1/2} \sin t (-\Delta)^{1/2} \delta_{(r_2, x_2)} \\ &= \frac{1}{\pi} (r_1 r_2)^{\alpha-1/2} \left\{ \log \frac{2}{\delta_1} \cos \pi v \delta_{x_2} \right. \\ & \quad \left. + \int_0^\pi \frac{\cos s v - \cos \pi v}{2 \cos \frac{1}{2}s} ds \delta_{x_2} + R_1 \delta_{x_2} \right\}, \end{aligned}$$

where, for $s > (m+1)/2$,

$$(8.109) \quad \|R_1 \delta_{x_2}\|_{\mathcal{D}^{-s-1}} \leq C \delta_1 \log \frac{1}{\delta_1}, \text{ as } \delta_1 \searrow 0.$$

The following result analyzes the second term on the right in (8.108).

Proposition 8.10. We have

$$(8.110) \quad \begin{aligned} & \int_0^\pi \left(2 \cos \frac{1}{2}s\right)^{-1} (\cos s v - \cos \pi v) ds \\ &= \cos \pi v \left\{ -\log v + \sum_{j=0}^K a_j v^{-2j} \right\} + \frac{\pi}{2} \sin \pi v + S_K(v), \end{aligned}$$

where $S_K(v) : \mathcal{D}^s \rightarrow \mathcal{D}^{s+2K}$, for all s .

The spaces \mathcal{D}^s are spaces of generalized functions on N , introduced in Chap. 5, Appendix A.

We turn to the analysis of v in region III. Using (8.91), we can write v as

$$(8.111) \quad \frac{1}{\pi} (r_1 r_2)^{\alpha-1/2} \cos \pi v Q_{v-1/2}(\cosh \beta_2) \delta_{x_2}, \quad \text{in region III,}$$

where $Q_{v-1/2}$ is the Legendre function given by (8.80) and β_2 is given by (8.92). It is more convenient to use (8.96) instead; this yields for v the formula

$$(8.112) \quad \begin{aligned} & \frac{1}{\pi} (r_1 r_2)^{\alpha-1/2} \left\{ \int_0^\pi (2 \cosh \beta_2 + 2 \cos s)^{-1/2} \cos s v ds \right. \\ & \quad \left. - \sin \pi v \int_0^{\beta_2} (2 \cosh \beta_2 - 2 \cosh s)^{-1/2} e^{-s v} ds \right\}. \end{aligned}$$

Note that as $r_1 \nearrow t - r_2$, $\beta_2 \searrow 0$.

The first integral in (8.112) has an analysis similar to that arising in (8.103); first replace s by $\pi - s$ to rewrite the integral as

$$(8.113) \quad \begin{aligned} & \cos \pi \nu \int_0^\pi (2 \cosh \beta_2 - 2 \cos s)^{-1/2} \cos s \nu \, ds \\ & + \sin \pi \nu \int_0^\pi (2 \cosh \beta_2 - 2 \cos s)^{-1/2} \sin s \nu \, ds. \end{aligned}$$

As $\beta_2 \searrow 0$, the second term in (8.113) tends to the limit (8.104), and the first term also has an analysis similar to (8.105)–(8.107), with (8.107) replaced by

$$(8.114) \quad \begin{aligned} & \int_0^\pi (2 \cosh \beta_2 - 2 \cos s)^{-1/2} \, ds \\ & \sim \left(\log \frac{2}{\beta_2} \right) \sum_{j \geq 0} A'_j \beta_2^j + \sum_{j \geq 1} B'_j \beta_2^j, \quad A'_0 = 1. \end{aligned}$$

It is the second term in (8.112) that leads to the jump across $r_1 = t - r_2$, hence to the diffracted wave. We have

$$(8.115) \quad \int_0^{\beta_2} (2 \cosh \beta_2 - 2 \cosh s)^{-1/2} e^{-s\nu} \, ds \sim \int_0^{\beta_2} \frac{ds}{\sqrt{\beta_2^2 - s^2}} = \frac{\pi}{2}.$$

Thus we have the following:

Proposition 8.11. *For $r_1 \nearrow t - r_2$,*

$$(8.116) \quad \begin{aligned} & (-\Delta)^{-1/2} \sin t (-\Delta)^{1/2} \delta_{(r_2, x_2)} \\ & = \frac{1}{\pi} (r_1 r_2)^{\alpha-1/2} \left\{ \log \frac{2}{\beta_2} \cos \pi \nu \, \delta_{x_2} \right. \\ & \quad \left. + \int_0^\pi \frac{\cos s \nu - \cos \pi \nu}{2 \cos \frac{1}{2}s} \, ds \, \delta_{x_2} - \frac{\pi}{2} \sin \pi \nu \, \delta_{x_2} + \widetilde{R}_1 \delta_{x_2} \right\}, \end{aligned}$$

where, for $s > (m+1)/2$,

$$(8.117) \quad \|R_1 \delta_{x_2}\|_{\mathcal{D}^{-s-1}} \leq C \beta_2 \log \frac{1}{\beta_2}, \quad \text{as } \beta_2 \searrow 0.$$

Note that (8.116) differs from (8.108) by the term $\pi^{-1} (r_1 r_2)^{\alpha-1/2}$ times

$$(8.118) \quad -\frac{\pi}{2} \sin \pi \nu \, \delta_{x_2}.$$

This contribution represents a jump in the fundamental solution across the diffracted wave \mathcal{D} . There is also the logarithmic singularity, $(r_1 r_2)^{\alpha-1/2}$ times

$$(8.119) \quad \frac{1}{\pi} \log \frac{2}{\delta} \cos \pi \nu \, \delta_{x_2},$$

where $\delta = \delta_1$ in (8.108) and $\delta = \beta_2$ in (8.116). In the special case where N is an interval $[0, L]$, so $\dim C(N) = 2$, $\cos \pi \nu \delta_{x_2}$ is a sum of two delta functions. Thus its manifestation in such a case is subtle.

We also remark that if N is a subdomain of the unit sphere S^{2k} (of *even* dimension), then $\cos \pi \nu \delta_{x_2}$ vanishes on the set $N \setminus N_0$, where

$$(8.120) \quad N_0 = \{x_1 \in N : \text{for some } y \in \partial N, \text{dist}(x_2, y) + \text{dist}(y, x_1) \leq \pi\}.$$

Thus the log blow-up disappears on $N \setminus N_0$. This follows from the fact that $\cos \pi \nu_0 = 0$, where ν_0 is the operator (8.46) on S^{2k} , together with a finite propagation speed argument.

While Propositions 8.9–8.11 contain substantial information about the nature of the diffracted wave, this information can be sharpened in a number of respects. A much more detailed analysis is given in [CT].

Exercises

- Using (7.36) and (7.80), work out the asymptotic behavior of ${}_1F_1(a; b; -z)$ as $z \rightarrow +\infty$, given $b, b-a \notin \{0, -1, -2, \dots\}$. Deduce from (8.51) that whenever $\nu \geq 0$, $s \in \mathbb{R}$,

$$(8.121) \quad \lim_{b \searrow 0} \int_0^\infty e^{-br^2} J_\nu(r) r^{-is} dr = 2^{-is} \frac{\Gamma(\frac{1}{2}(\nu + 1 - is))}{\Gamma(\frac{1}{2}(\nu + 1 + is))}.$$

- Define operators

$$(8.122) \quad M_r f(r) = r f(r), \quad \mathcal{J} f(r) = f(r^{-1}).$$

Show that

$$(8.123) \quad \begin{aligned} M_r : L^2(\mathbb{R}^+, r dr) &\longrightarrow L^2(\mathbb{R}^+, r^{-1} dr), & \mathcal{J} : L^2(\mathbb{R}^+, r^{-1} dr) \\ &\longrightarrow L^2(\mathbb{R}^+, r^{-1} dr) \end{aligned}$$

are unitary. Show that

$$(8.124) \quad H_\nu^\# = \mathcal{J} M_r H_\nu M_r^{-1}$$

is given by

$$(8.125) \quad H_\nu^\# f(\lambda) = (f \star \ell_\nu)(\lambda),$$

where \star denotes the natural convolution on \mathbb{R}^+ , with Haar measure $r^{-1} dr$:

$$(8.126) \quad (f \star g)(\lambda) = \int_0^\infty f(r) g(r^{-1} \lambda) r^{-1} dr,$$

and

$$(8.127) \quad \ell_\nu(r) = r^{-1} J_\nu(r^{-1}).$$

3. Consider the Mellin transform:

$$(8.128) \quad \mathcal{M}^\# f(s) = \int_0^\infty f(r) r^{is-1} dr.$$

As shown in (A.17)–(A.20) of Chap. 3, we have

$$(8.129) \quad (2\pi)^{-1/2} \mathcal{M}^\# : L^2(\mathbb{R}^+, r^{-1} dr) \longrightarrow L^2(\mathbb{R}, ds), \text{ unitary.}$$

Show that

$$(8.130) \quad \mathcal{M}^\#(f \star g)(s) = \mathcal{M}^\# f(s) \cdot \mathcal{M}^\# g(s),$$

and deduce that

$$(8.131) \quad \mathcal{M}^\# H_\nu^\# f(s) = \Psi(s) \mathcal{M}^\# f(s),$$

where

$$(8.132) \quad \Psi(s) = \int_0^\infty J_\nu(r^{-1}) r^{is-2} dr = \int_0^\infty J_\nu(r) r^{-is} dr = 2^{-is} \frac{\Gamma(\frac{1}{2}(\nu + 1 - is))}{\Gamma(\frac{1}{2}(\nu + 1 + is))}.$$

4. From (8.126)–(8.132), give another proof of the unitarity (8.13) of H_ν . Using symmetry, deduce that $\text{spec } H_\nu = \{-1, 1\}$, and hence deduce again the inversion formula (8.14).

5. Verify the asymptotic expansion (8.107). (*Hint*: Write $2 \cos \delta - 2 \cos s = (s^2 - \delta^2) F(s, \delta)$ with F smooth and positive, $F(0, 0) = 1$. Then, with $G(s, \delta) = F(s, \delta)^{-1/2}$,

$$(8.133) \quad \int_\delta^\pi (2 \cos \delta - 2 \cos s)^{-1/2} ds = \int_\delta^\pi G(s, \delta) \frac{ds}{\sqrt{s^2 - \delta^2}}.$$

Write $G(s, \delta) = g(s) + \delta H(s, \delta)$, $g(0) = 1$, and verify that (8.133) is equal to $A_1 + A_2$, where

$$A_1 = \int_\delta^\pi G(s, \delta) \frac{ds}{s} = g(0) \log \frac{1}{\delta} + O\left(\delta \log \frac{1}{\delta}\right),$$

$$A_2 = \int_\delta^\pi g(s) \left[\frac{1}{\sqrt{s^2 - \delta^2}} - \frac{1}{s} \right] ds + O(\delta) = B_2 + O(\delta).$$

Show that

$$B_2 = g(0) \int_1^{\pi/\delta} \left[\frac{1}{\sqrt{t^2 - 1}} - \frac{1}{t} \right] dt + O(\delta) = C_2 + O(\delta),$$

with

$$C_2 = \int_1^\infty \left[\frac{1}{\sqrt{t^2 - 1}} - \frac{1}{t} \right] dt$$

Use the substitution $t = \cosh u$ to do this integral and get $C_2 = \log 2$.)

Next, verify the expansion (8.114).

Exercises on the hypergeometric function

1. Show that ${}_2F_1(a_1, a_2; b; z)$, defined by (8.56), satisfies

$$(8.134) \quad {}_2F_1(a_1, a_2; b; z) = \frac{\Gamma(b)}{\Gamma(a_2)\Gamma(b-a_2)} \int_0^1 t^{a_2-1} (1-t)^{b-a_2-1} (1-tz)^{-a_1} dt,$$

for $\operatorname{Re} b > \operatorname{Re} a_2 > 0$, $|z| < 1$. (*Hint*: Use the beta function identity, (A.23)–(A.24) of Chap. 3, to write

$$\frac{(a_2)_k}{(b)_k} = \frac{\Gamma(b)}{\Gamma(a_2)\Gamma(b-a_2)} \int_0^1 t^{a_2-1+k} (1-t)^{b-a_2-1} dt, \quad k = 0, 1, 2, \dots,$$

and substitute this into (8.39). Then use

$$\sum_{k=0}^{\infty} \frac{(a_1)_k}{k!} (zt)^k = (1-tz)^{-a_1}, \quad 0 \leq t \leq 1, \quad |z| < 1.$$

2. Show that, given $\operatorname{Re} b > \operatorname{Re} a_2 > 0$, (8.134) analytically continues in z to $z \in \mathbb{C} \setminus [1, \infty)$.
 3. Show that the function (8.134) satisfies the ODE

$$z(1-z) \frac{d^2 u}{dz^2} + \{b - (a_1 + a_2 + 1)z\} \frac{du}{dz} - a_1 a_2 u = 0$$

Note that $u(0) = 1$, $u'(0) = a_1 a_2 / b$, but zero is a singular point for this ODE. Show that another solution is

$$u(z) = z^{1-b} {}_2F_1(a_1 - b + 1, a_2 - b + 1; 2 - b; z).$$

4. Show that

$${}_2F_1(a_1, a_2; b; z) = (1-z)^{-a_1} {}_2F_1(a_1, b-a_2; b; (z-1)^{-1}z).$$

(*Hint*: Make a change of variable $s = 1 - t$ in (8.134).)

For many other important transformation formulas, see [Leb] or [WW].

5. Show that

$${}_1F_1(a; b; z) = \lim_{c \nearrow \infty} {}_2F_1(a, c; b; c^{-1}z).$$

We mention the generalized hypergeometric function, defined by

$${}_pF_q(a; b; z) = \sum_{k=0}^{\infty} \frac{(a)_k}{(b)_k} \frac{z^k}{k!},$$

where $p \leq q + 1$, $a = (a_1, \dots, a_p)$, $b = (b_1, \dots, b_q)$, $b_j \in \mathbb{C} \setminus \{0, -1, -2, \dots\}$, $|z| < 1$, and

$$(a)_k = (a_1)_k \cdots (a_p)_k, \quad (b)_k = (b_1)_k \cdots (b_q)_k,$$

and where, as before, for $c \in \mathbb{C}$, $(c)_k = c(c+1) \cdots (c+k-1)$. For more on this class of functions, see [Bai].

6. The Legendre function $Q_{\nu-1/2}(z)$ satisfies the identity (8.87), for $\nu \geq 0$, $|z| > 1$, and $|\arg z| < \pi$; cf. (7.3.7) of [Leb]. Take $z = (r_1^2 + r_2^2 + t^2)/2r_1r_2$, and compare the resulting power series for the right side of (8.77) with the power series in (8.76).

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