Sturm–Liouville operators

Our study is motivated by the following fundamental problem, adapted from Fourier's [Fou].

The heated bar. Let the bar be given by the interval $[0,1]$. Let $u(x,t)$ denote the temperature at position x and time t. Let $h(x)$ denote the intial temperature distribution, i.e.

$$u(x,0) = h(x).$$

The rate of change of the total heat in any subinterval $[a,x] \subset [0,1]$ is equal to the flux F of heat into the endpoints of the interval:

$$\partial_t \int_a^x u(y,t)\,dy = F(a,t) - F(x,t).$$

Differentiating with respect to x gives

$$\partial_t u(x,t) = -\partial_x F(x,t). \tag{1}$$

Under reasonable conditions, heat flows from hotter regions to colder ones at a rate proportional to the temperature gradient:

$$F(x,t) = -\kappa(x)\partial_x u(x,t), \tag{2}$$

where the constant of proportionality $\kappa(x) > 0$ depends on properties of the bar at the position x. Plugging (2) into (1) yields the *heat equation*

$$\partial_t u(x,t) = \partial_x\Big(\kappa(x)\partial_x u(x,t)\Big).$$

At the ends of the interval, we consider two kinds of conditions. The condition

$$u(0,t) = u(1,t) = 0,$$

called the *Dirichlet condition*, corresponds to the temperature at the ends being held fixed at 0. The condition

$$\partial_x u(0,t) = \partial_x u(1,t) = 0,$$

called the *Neumann condition*, corresponds to the flux at the ends being held fixed at 0, i.e. the ends being insulated so that no heat can flow in or out.

This problem is solved by separation of variables. In Hilbert space terms, we seek an orthonormal basis $e_1(x),\ e_2(x),\ \dots$ of $L^2(0,1)$ and numbers $\lambda_1,\ \lambda_2,\ \dots$ such that

$$-(\kappa(x)e_j'(x))' = \lambda_j e_j(x),$$

and such that

$$e_j(0) = e_j(1) = 0, \qquad \text{or} \qquad e_j'(0) = e_j'(1) = 0,$$

for the Dirichlet or Neumann conditions respectively. The basic examples are when $\kappa = 1$ and we get Fourier sine and cosine series:

$$e_j(x) = \frac{1}{\sqrt{2}}\begin{cases}\sin(j\pi x), & \text{Dirichlet}, \\ \cos(j\pi x), & \text{Neumann},\end{cases} \qquad \lambda_j = j^2\pi^2, \tag{3}$$

where in the Neumann case we must also include another basis vector $e_0(x) = 1$ and corresponding eigenvalue $\lambda_0 = 0$; this can be derived by projecting the basis $(\exp(ik\pi x))_{k\in\mathbb{Z}}$ for $L^2(-1,1)$ onto the odd (for Dirichlet) or even (for Neumann) subspaces of $L^2(-1,1)$, and then mapping to $L^2(0,1)$.

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Whenever we have such a basis, provided $\lim_{j\to\infty}\lambda_j=\infty$, we can write

$$h(x)=\sum_{j=1}^\infty c_j e_j(x), \qquad c_j=\langle e_j,h\rangle_{L^2},$$

and put

$$u(x,t)=\sum_{j=1}^\infty c_j e^{-t\lambda_j}e_j(x).$$

More abstractly, we say that we are solving

$$\partial_t u(x,t)=-Au(x,t), \qquad u(x,0)=h(x),$$

by putting

$$u(x,t)=e^{-tA}h(x),$$

with e^{-tA} defined by the *eigenbasis functional calculus*:

$$\varphi(A)\sum_{j=1}^\infty c_j e_j=\sum_{j=1}^\infty c_j\varphi(\lambda_j)e_j.$$

Note that even though $A=-\frac{d}{dx}\kappa(x)\frac{d}{dx}$ is an unbounded operator, $\varphi(A)$ is bounded whenever φ is bounded on the spectrum, and this applies to $\varphi(A)=e^{-tA}$ as long as $\lim_{j\to\infty}\lambda_j=\infty$.

To check that such an eigenbasis exists, we need the following ODE existence and uniqueness theorem, for the proof of which we follow Section 5.1 of [Olv].

Definition. For $\alpha<\beta$ real numbers, $k\in\mathbb{N}$, the Sobolev space $H^k(\alpha,\beta)$ is the set of $u\in C^{k-1}([\alpha,\beta])$ for which there exist $v\in L^2(\alpha,\beta)$ and a constant c such that $u^{(k-1)}(x)=c+\int_\alpha^x v$. We also put $H^0(\alpha,\beta)=L^2(\alpha,\beta)$.

Exercise 1. Let γ be a real number, $u(x)=|x|^\gamma$. For which k is $u\in H^k(-1,1)$?

Theorem 1. *For any $a,b\in L^\infty(0,1)$, and $\alpha,\beta\in\mathbb{C}$, there is a unique $u\in W^{2,\infty}(0,1)$ which solves*

$$u''(x)+a(x)u'(x)+b(x)u(x)=0, \qquad u'(0)=\alpha,\ u(0)=\beta. \tag{4}$$

Proof. Without loss of generality, we may assume that (α,β) is $(1,0)$ or $(0,1)$.

Integrating (4) yields

$$u'(x)=-\int_0^x\Big(a(y)u'(y)-b(y)u(y)\Big)\,dy+\alpha$$

Integrating again, and integrating by parts to simplify, gives

$$u(x)=\int_0^x(y-x)\Big(a(y)u'(y)+b(y)u(y)\Big)\,dy+\alpha x+\beta. \tag{5}$$

So if u solves (4) then it solves (5). Conversely, direct calculation shows that if u solves (5) then it solves (4).

To solve (5), put

$$\varphi_0(x)=\alpha x+\beta, \qquad \varphi_{n+1}(x)=\int_0^x(y-x)\Big(a(y)\varphi_n'(y)+b(y)\varphi_n(y)\Big)\,dy, \qquad u(x)=\sum_{n=0}^\infty\varphi_n(x).$$

To check convergence of the sum, estimate

$$|\varphi_1(x)| = \Big| \int_0^x (y-x)\Big(a(y)\alpha + b(y)(\alpha y + \beta)\Big)\, dy\Big| \leq Mx,$$

where $M = \|a\|_{L^\infty} + \|b\|_{L^\infty}$. Similarly,

$$|\varphi_1'(x)| = \Big| \int_c^x \Big(a(y)\alpha + b(y)(\alpha y + \beta)\Big)\, dy\Big| \leq Mx.$$

Inductively, if

$$|\varphi_n(x)| \leq \frac{(Mx)^n}{n!}, \qquad |\varphi_n'(x)| \leq \frac{(Mx)^n}{n!},$$

then

$$|\varphi_{n+1}(x)| = \Big| \int_0^x (y-x)(a(y)\varphi_n'(y) + b(y)\varphi_n(y))\, dy\Big| \leq \frac{M^{n+1}}{n!}\int_0^x y^n\, dy = \frac{(Mx)^{n+1}}{(n+1)!},$$

and similarly for φ_{n+1}'. Uniqueness is proved in Exercise 2. □

Exercise 2. Let u_1 and u_2 be any two solutions to (4), and let $w = u_1 - u_2$. Prove that w is identically zero by using the integral equation obeyed by w (a version of (5)) to show that $|w(x)| \leq (2Mx)^n/n!$ for any n.

Now we are ready to prove that an eigenbasis exists, as in the Supplement to VI.5 of [ReSi].

Theorem 2. *Let $\kappa \in C^1([0,1])$, $V \in L^\infty(0,1)$, with κ positive and V real valued. Let*

$$\mathcal{D} = \{u \in H^2(0,1)\colon u(0) = u(1) = 0\}, \qquad \text{or} \qquad \mathcal{D} = \{u \in H^2(0,1)\colon u'(0) = u'(1) = 0\}.$$

Let

$$A\colon \mathcal{D} \to L^2(0,1), \qquad Au = (-\kappa u')' + Vu.$$

There exists an orthonormal basis $e_1, e_2 \dots$ of $L^2(0,1)$, and a corresponding sequence of real numbers $\lambda_1 < \lambda_2 < \cdots$, such that $\lambda_j \to \infty$, each e_j is in $\mathcal{D}$, and

$$Ae_j = \lambda_j e_j. \tag{6}$$

For our application to the heated bar problem we take $V = 0$, but for other applications, such as to quantum mechanics, it is interesting to take nontrivial V, and we will see that this makes essentially no difference to the proof. [1]

Proof. We define the λ_j to be those complex numbers for which we can solve (6) for some $e_j \in \mathcal{D}$ with $\|e_j\|_{L^2(0,1)} = 1$. By uniqueness of solutions to ODEs (Theorem 1), if $\tilde{e}_j$ is a second solution to (6) with the same λ_j, then e_j and $\tilde{e}_j$ are proportional. Thus we say that each λ_j is a *simple* eigenvalue.

By integration by parts,

$$\lambda_j = \lambda_j \int_0^1 |e_j|^2 = \int_0^1 \overline{e_j}\Big(-(\kappa e_j')' + Ve_j\Big) = \int_0^1 \Big(\kappa|e_j'|^2 + V|e_j|^2\Big) \geq \int_0^1 V|e_j|^2 \geq \operatorname{ess\,inf} V, \tag{7}$$

so all the λ_j are real and bounded below. Moreover, if $\lambda_j \neq \lambda_k$, then e_j and e_k are orthogonal, because the same integration by parts calculation shows $\lambda_k \int \overline{e_j} e_k = \lambda_j \int \overline{e_j} e_k$. Since $L^2(0,1)$ is separable, this shows that the λ_j are at most countable. Let $S = \{\lambda_1, \lambda_2, \dots\}$.

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[1] See Chapter 9 of [Tes] for a more general treatment. Another possible variant is to replace $(0,1)$ by an unbounded interval and require $V \to \infty$ as $|x| \to \infty$.

It remains to show that the e_1, e_2, ... have dense span in $L^2(0,1)$. This is the hard part. (At this point we have not even shown that S is nonempty.) For this we will construct the resolvent $(A-\lambda)^{-1}$: given $f \in L^2(0,1)$ and $\lambda \notin S$, we will solve

$$(A-\lambda)u = f. \tag{8}$$

for $u \in \mathcal{D}$.

Observe first that a solution to (8), if it exists, is unique. Indeed, the difference of any two solutions is in the kernel of $(A-\lambda)$ and hence vanishes because $\lambda \notin S$.

By the method of variation of parameters, we look for a solution to (8) of the form

$$u(x) = \int_0^1 G(x,y) f(y)\, dy, \tag{9}$$

where

$$G(x,y) = -\frac{u_0(\min(x,y))u_1(\max(x,y))}{\kappa W}, \tag{10}$$

where u_0 and u_1 are solutions to the homogeneous equation

$$-(\kappa u')' + Vu - \lambda u = 0, \tag{11}$$

and $W = u_0' u_1 - u_0 u_1'$ is their Wronskian. Note that $(\kappa W)' = 0$, so the denominator in (10) is constant and nonzero as long as u_0 and u_1 are linearly independent.

A direct calculation shows that u, defined by (9), solves (8). It remains to fix the boundary conditions, i.e. to get $u \in \mathcal{D}$. For this we impose

$$u_0(0) = u_1(1) = 0, \qquad \text{or} \qquad u_0'(0) = u_1'(1) = 0, \tag{12}$$

according to which boundary conditions we are considering. This is consistent with $\kappa W \neq 0$, because if u_0 and u_1 were linearly dependent and nonzero, then they would be eigenfunctions and this is ruled out by $\lambda \notin S$.

We have now proven that $(A-\lambda)\colon \mathcal{D} \to L^2(0,1)$ is invertible for $\lambda \notin S$, and

$$\Big((A-\lambda)^{-1} f\Big)(x) = \int_0^1 G(x,y) f(y)\, dy.$$

Since G is continuous, $(A-\lambda)^{-1}$ is compact for all $\lambda \notin S$. Moreover, if λ is real then we may choose u_0 and u_1 real valued, which, combined with $G(x,y) = G(y,x)$, yields

$$\int_0^1 \overline{g(x)} \int_0^1 G(x,y) f(y)\, dy\, dx = \int_0^1 \int_0^1 \overline{G(y,x) g(x)}\, dx f(y)\, dy,$$

and hence $(A-\lambda)^{-1}$ is self-adjoint on $L^2(0,1)$ for $\lambda \in \mathbb{R} \setminus S$.

Fix $\Lambda \in \mathbb{R} \setminus S$ and let $R = (A-\Lambda)^{-1}$. Since the eigenvectors of R have dense span in $L^2(0,1)$, it is enough to prove that R has the same eigenvectors as A. For this, observe that 0 is not an eigenvalue of R because $(A-\Lambda)R = I$, while for $\mu \neq 0$, we have $\ker(R-\mu) = \ker(A - \Lambda - \mu^{-1})$. □

The eigenfunction e_1 is called the *ground state*, and λ_1 is the *ground state energy*. Note that if V is identically zero, as in the original heated bar problem, then our integration by parts calculation (7) shows that $\lambda_1 \geq 0$. Equality occurs if and only if the boundary condition is Neumann, and in that case e_1 is constant. This shows that in the Dirichlet case we have

$$\int_0^1 |u(x,t)|^2\,dx = \int_0^1 \Big|\sum_{j=1}^\infty c_j e^{-t\lambda_j} e_j(x)\Big|^2\,dx = \sum_{j=1}^\infty |c_j|^2 e^{-2t\lambda_j} \leq e^{-2t\lambda_1}\sum_{j=1}^\infty |c_j|^2 = e^{-2t\lambda_1}\|h\|^2_{L^2(0,1)},$$

and so u converges to zero at an exponential rate, with the exponent given by the ground state energy.

Exercise 3. Prove that for the Neumann heated bar problem, u converges to a constant at an exponential rate. Give a simple formula for the constant in terms of the initial condition.

These examples demonstrate the importance of the lowest eigenvalues λ_1, λ_2. The best way to study these is the *variational method*. This has many far-reaching versions and generalizations (see Sections 5.4 and 6.4 of [Bor] for some of them) but a convenient basic one for our present setting is the following.

Theorem 3. *Let $A\colon \mathcal{D}\to\mathcal{H}$, with $\mathcal{D}\subset\mathcal{H}$, $e_1, e_2, \dots$ a sequence in $\mathcal{D}$ which is an orthonormal basis of $\mathcal{H}$, such that $Ae_j = \lambda_j e_j$, and such that $\lambda_1 = \min\{\lambda_1,\lambda_2,\dots\}$. Then*

$$\lambda_1 = \min_{u\in\mathcal{D}\setminus\{0\}} \frac{\langle u, Au\rangle_{\mathcal{H}}}{\|u\|^2_{\mathcal{H}}}.$$

Proof. Writing $u = \sum_{j=1}^\infty c_j e_j$, we have

$$\langle u, Au\rangle_{\mathcal{H}} = \sum_{j=1}^\infty \lambda_j |c_j|^2 \geq \lambda_1 \sum_{j=1}^\infty |c_j|^2 = \lambda_1\|u\|^2_{\mathcal{H}},$$

with equality when $u = e_j$. □

The quantity $\langle u, Au\rangle_{\mathcal{H}}/\|u\|^2_{\mathcal{H}}$ is called the *Rayleigh quotient*. For our heated bar, the integration by parts calculation (7) shows that it is given by

$$\frac{\langle u, Au\rangle_{\mathcal{H}}}{\|u\|^2_{\mathcal{H}}} = \frac{\int_0^1 \kappa|u'|^2}{\int_0^1 |u|^2}.$$

Thus if $\kappa(x)$ is between $\kappa_{\min}$ and $\kappa_{\max}$ for all x, then λ_1 for κ is between the λ_1's for $\kappa_{\min}$ and $\kappa_{\max}$, i.e. in the Dirichlet case we have

$$\kappa_{\min}\pi^2 \leq \lambda_1 \leq \kappa_{\max}\pi^2.$$

Applying Theorem 3 with $\mathcal{H}$ given by the orthogonal complement of the constant functions in $L^2(0,1)$ in the Neumann case we find the same result, where λ_1 now denotes the *second eigenvalue* (we start the indexing with λ_0 as in (3)).

Exercise 4. Let $A\colon\mathcal{D}\to\mathcal{H}$, $\mathcal{D}\subset\mathcal{H}$. Prove that the following are equivalent.

(1) There exist a sequence $e_1, e_2, \dots$ in $\mathcal{D}$ which is an orthonormal basis of $\mathcal{H}$, such that $Ae_j = \lambda_j e_j$, each λ_j is a real number, and $|\lambda_j|\to\infty$ as $j\to\infty$.
(2) There exists $\Lambda\in\mathbb{R}$ such that $(A-\Lambda)\colon\mathcal{D}\to\mathcal{H}$ is bijective, and $\imath(A-\Lambda)^{-1}\colon\mathcal{H}\to\mathcal{H}$ is compact and self-adjoint, where $\imath$ denotes the inclusion $\mathcal{D}\to\mathcal{H}$.

An operator with the properties in the Exercise above is called a *self-adjoint operator with compact resolvent*.

To put this in the more general context of unbounded operators on Hilbert space, we need some standard definitions as in Chapter 3 of [Bor] and Chapter VIII of [ReSi]. The *adjoint* of an operator $A\colon \mathcal{D}(A) \to \mathcal{H}$, where $\mathcal{D}(A) \subset \mathcal{H}$ is dense, is the operator $A^*\colon \mathcal{D}(A^*) \to \mathcal{H}$, where

$$\mathcal{D}(A^*) = \{\varphi \in \mathcal{H}\colon \text{ there exists } C_\varphi \text{ such that } |\langle \varphi, Au\rangle_{\mathcal{H}}| \le C_\varphi \|u\|_{\mathcal{H}} \text{ for all } u \in \mathcal{D}(A)\},$$

and where $A^*\varphi$ is defined by the Riesz representation theorem to be the unique element of $\mathcal{H}$ such that $\langle \varphi, Au\rangle_{\mathcal{H}} = \langle A^*\varphi, u\rangle_{\mathcal{H}}$ for all $u \in \mathcal{D}(A)$. An operator is *self-adjoint* if $A = A^*$.

A basic example is the multiplication operator $M_V\colon L^\infty(0,1) \to L^2(0,1)$, where V is measurable. Then $\mathcal{D}(M_V) = \mathcal{D}(M_V^*) = \{u \in L^2\colon Vu \in L^2\}$, with the domain being dense because it includes all simple functions, and $(M_V)^* = (M_{\bar V})^*$. So such an operator is self-adjoint if and only if V is real valued.

The definition of adjoint is cumbersome, but works well in the usual proof that

$$\ker A^* = (\operatorname{ran} A)^\perp, \tag{13}$$

which is enough for the following theorem.

Theorem 4. *The operator A from Theorem 2 is self-adjoint, in both the Dirichlet and Neumann cases.*

Proof. Observe first that, if $\varphi, u \in \mathcal{D}$, then the integration by parts calculation (7) implies that $\langle \varphi, Au\rangle_{L^2} = \langle A\varphi, u\rangle_{L^2}$. This shows that $\mathcal{D}(A) \subset \mathcal{D}(A^*)$ (using $C_\varphi = \|A\varphi\|_{L^2}$) and that A^* restricted to $\mathcal{D}(A)$ equals A.

It remains to show that $\mathcal{D}(A^*) \subset \mathcal{D}(A)$. Let $\varphi \in \mathcal{D}(A^*)$, let $\lambda \in \mathbb{C} \setminus S$, and let

$$u = (A - \lambda)^{-1}(A^* - \lambda)\varphi.$$

Then $(A - \lambda)u = (A^* - \lambda)\varphi$, and since $Au = A^*u$, we have $(A^* - \lambda)(u - \varphi) = 0$, so by (13) we have $u - \varphi \in (\operatorname{ran}(A - \bar\lambda))^\perp$. But since $\bar\lambda \in \mathbb{C} \setminus S$, this implies $u = \varphi$ because $(A - \bar\lambda)\colon \mathcal{D}(A) \to L^2$ is bijective. □

When $\mathcal{D}(A) \subset \mathcal{D}(A^*)$ and $A^*|_{\mathcal{D}(A)} = A$, as in the first paragraph of the above proof, we say that A is *symmetric*. This pattern of analysis is typical for self-adjoint differential operators: one proves relatively easily by integration by parts that the operator is symmetric, and then works harder to establish self-adjointness.

Let us now give another more abstract proof that A as in Theorem 2 has compact resolvent, one which generalizes to higher dimensional domains and manifolds.

For this, we use the fact that $H^1(0,1)$ is a Hilbert space for the inner product

$$\langle f, g\rangle_{H^1} = \langle f, g\rangle_{L^2} + \langle f', g'\rangle_{L^2}.$$

Indeed, H^1 is a closed subspace of the direct sum of L^2 with itself.

For the Dirichlet problem, we work with

$$H^1_0 = \{u \in H^1\colon u(0) = u(1) = 0\},$$

which is a closed subspace of H^1.

Theorem 5. *If $\lambda < \operatorname{ess\,inf} V$, then $(A-\lambda)\colon H^2 \cap H_0^1 \to L^2$ is bijective.*

Proof. First note that the domain and codomain are correct, and the map is injective.

To prove surjectivity, for $f,\, g \in H_0^1$, let

$$Q(f,g) = \int_0^1 \Big(\kappa \overline{f}' g' + (V-\lambda)\overline{f} g\Big).$$

If $\lambda <$ ess inf V, then Q defines an inner product on H_0^1 with an equivalent norm to that of the $\langle\cdot,\cdot\rangle$ inner product. Then, similarly to (7), for all $u \in \mathcal{D}$ and $\varphi \in H_0^1(0,1)$, we have

$$\langle \varphi, (A-\lambda)u\rangle_{L^2} = Q(\varphi, u). \tag{14}$$

By the Riesz representation theorem, given $f \in L^2$, there is a unique $u \in H_0^1$ such that

$$\langle \varphi, f\rangle_{L^2} = Q(\varphi, u)$$

for all $\varphi \in H_0^1$. Next, we check that $u \in H^2$; this holds because, by (14), $\kappa u'$ has a weak derivative obeying

$$-(\kappa u')' + (V-\lambda)u = f;$$

see Section 2.5 of [Bor]. □

This proof generalizes directly to higher dimensions and manifolds. Let $\Omega \subset \mathbb{R}^d$ be an open set (or a Riemannian manifold) and define $A\colon \{u \in H_0^1(\Omega)\colon \operatorname{div}(\kappa \text{ grad } u) \in L^2(\Omega)\} \to L^2(\Omega)$ by

$$A = -\operatorname{div}(\kappa \text{ grad } u) + Vu,$$

and put

$$Q(f,g) = \int_\Omega \kappa |\text{grad } u|^2 + V|u|^2.$$

Next prove compactness by proving compactness of the inclusion $H_0^1(\Omega) \to L^2(\Omega)$ when Ω is bounded. For this, factorize this inclusion as a composition

$$H_0^1(\Omega) \to H^1(\mathbb{T}) \to L^2(\mathbb{T}) \to L^2(\Omega),$$

where $\mathbb{T}$ is a torus that contains Ω (on a manifold, use a partition of unity and local coordinates as in Section 9.4 of [Bor]), and prove compactness of the middle term using Fourier series as in Section 6.2.1 of [Bor]).

Unbounded domains. Now consider the operator

$$Au = -(\kappa u')' + Vu = 0,$$

where $\kappa \in C^1(\mathbb{R})$, $V \in L^\infty(\mathbb{R})$, $\kappa > 0$, and such that $(\kappa - 1)$ and V are both compactly supported. We equip A with the domain

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

Let us see how Stone's formula ([Bor, Theorem 5.10] or [ReSi, Theorem VII.13])

$$g(A) = \frac{1}{2\pi i} \lim_{\varepsilon \to 0^+} \int_{-\infty}^{\infty} g(\lambda) \Big[(A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1}\Big]\, d\lambda \tag{15}$$

simplifies in this example, following in part [TaZw].

As in (10), we solve

$$(A-\lambda)u = f,$$

by writing

$$u(x) = \int_{-\infty}^{\infty} G(x,y) f(y)\, dy,$$

with

$$G(x,y) = -\frac{u_-(\min(x,y))u_+(\max(x,y))}{\kappa W},$$

where u_- and u_+ are solutions to the homogeneous equation

$$-(\kappa u')' + Vu - \lambda u = 0.$$

We put $k = \sqrt{\lambda}$, with $\operatorname{Im} k > 0$ when $\lambda \notin [0,\infty)$, and impose

$$u_-(x) = e^{-ikx}, \qquad \text{when } x \ll 0,$$

and

$$u_+(x) = e^{ikx}, \qquad \text{when } x \gg 0.$$

Correspondingly, there are complex constants A_k, B_k, C_k, D_k such that

$$u_-(x) = A_k e^{-ikx} + B_k e^{ikx}, \qquad \text{when } x \gg 0,$$

and

$$u_+(x) = C_k e^{-ikx} + D_k e^{ikx}, \qquad \text{when } x \ll 0.$$

Since u_+ and u_- are continuous, it follows that there is $c(k)$ such that for all real x we have

$$|u_-(x)| \le c(k) e^{\operatorname{Im}(k)x}, \qquad |u_+(x)| \le c(k) e^{-\operatorname{Im}(k)x}.$$

Hence

$$|G(x,y)| \le c'(k) e^{\operatorname{Im}(k)\min(x,y)} e^{-\operatorname{Im}(k)\max(x,y)} = c'(k) e^{-\operatorname{Im}(k)|x-y|},$$

so, by Schur's test (Exercise 2.11 of [Bor]), G defines a bounded on operator on $L^2(\mathbb{R})$. Thus we have solved

$$(A - \lambda)u = f,$$

as long as $\lambda \notin [0,\infty)$ and $W \neq 0$; note that as before $W = 0$ is equivalent to λ being an eigenvalue of A. Also as before, A is symmetric by integration by parts, so it is self-adjoint and any eigenvalues can only be real and negative. Moreover, if λ_j is an eigenvalue with normalized eigenfunction e_j, then

$$\lambda_j = \int_{-\infty}^{\infty} \kappa |e_j'|^2 + V|e_j|^2 \ge \operatorname{essinf} V,$$

and since the Wronskian is entire in k, it follows that there can be only finitely many eigenvalues, all in the interval $[\operatorname{essinf} V, 0)$.

To get the contribution of an eigenvalue λ_j to (15), we write

$$\frac{1}{2\pi i} \lim_{\varepsilon \to 0^+} \int_{\lambda_j - \delta}^{\lambda_j + \delta} g(\lambda) \Big[(A - \lambda - i\varepsilon)^{-1} - (A - \lambda + i\varepsilon)^{-1} \Big]\, d\lambda = -g(\lambda_j) \frac{1}{2\pi i} \int_{\Gamma_{\lambda_j}} (\lambda - A)^{-1}\, d\lambda,$$

where Γ_{λ_j} is a small loop about λ_j, because we may take the limit as $\delta \to 0$ (since the two resolvents in the integrand on the left cancel for λ in a punctured neighborhood of λ_j). Thus we must compute a residue. The integral kernel $G(x,y)$ has a simple pole (a pole of higher order would contradict the resolvent bound $\|(A-\lambda)^{-1}\|_{\mathcal{H}\to\mathcal{H}} = \sup_{x\in\sigma(A)} |x-\lambda|^{-1} \le \sup_{x\in\mathbb{R}} |x-\lambda|^{-1} = |\operatorname{Im}\lambda|^{-1} \le |\lambda - \lambda_j|^{-1}$), and at this pole $k = i\mu_j$ with $\mu_j = \sqrt{-\lambda_j} > 0$ and each of u_+, u_- is a multiple of a corresponding normalized eigenfunction e_j, yielding that the integral kernel of

$$-g(\lambda_j) \frac{1}{2\pi i} \int_{\Gamma_{\lambda_j}} (\lambda - A)^{-1}\, d\lambda$$

is

$$g(\lambda_j)e_j(x)e_j(y),$$

since when g is the indicator function of λ_j we must get a projection by the functional calculus (the multiplier of an indicator function is a projection). Hence we may write (15) as

$$\big[g(A)\big](x,y) = \sum_{j=1}^{J} g(\lambda_j)e_j(x)e_j(y) + \frac{1}{2\pi i}\int_0^\infty g(\lambda)\Big[G_{k(\lambda)}(x,y) - G_{-k(\lambda)}(x,y)\Big]\,d\lambda,$$

or

$$\big[g(A)\big](x,y) = \sum_{j=1}^{J} g(\lambda_j)e_j(x)e_j(y) + \frac{1}{\pi i}\int_0^\infty g(k^2)\Big[G_k(x,y) - G_{-k}(x,y)\Big]k\,dk. \tag{16}$$

Note that for the free problem $A_0 = -\frac{d^2}{dx^2}$ we have, by Fourier transformation,

$$g(A_0)(x,y) = \frac{1}{2\pi}\int_{-\infty}^\infty g(k^2)e^{ik(x-y)}\,dk = \frac{1}{2\pi}\int_0^\infty g(k^2)\Big[e^{-ikx}e^{iky} + e^{ikx}e^{-iky}\Big]\,dk.$$

Thus,

$$g(A_0)u = \int_0^\infty dk\, g(k^2)\Big[\langle e_{-k}, u\rangle_{L^2(\mathbb{R})}\, e_{-k} + \langle e_k, u\rangle_{L^2(\mathbb{R})}\, e_k\Big], \qquad e_k(x) = e^{ikx}/\sqrt{2\pi}, \tag{17}$$

which is to be compared with the formula

$$g(B)u = \sum_{j=1}^{\infty} g(\lambda_j)\langle e_j, u\rangle_{\mathcal{H}}\, e_j. \tag{18}$$

for discrete spectrum. We say that in (17) the continuous spectrum $[0,\infty)$ has multiplicity two, because there are two terms. If we did the same problem with $\mathbb{R}$ replaced by the half line, with a Dirichlet or Neumann boundary condition at 0, we would get just one term.

We also write (18) as

$$g(B) = \sum_{j=1}^{\infty} g(\lambda_j)e_j \otimes e_j,$$

where $\otimes$ is the tensor product, or outer product, (in Dirac's notation $v \otimes w = |v\rangle\langle w|$) and similarly (17) as

$$g(A_0) = \int_0^\infty dk\, g(k^2)\Big[e_{-k}\otimes e_{-k} + e_k \otimes e_k\Big].$$

To get the same result for A, we use Vodev's identity to derive scattering solutions, and get

$$g(A) = \sum_{j=1}^{J} g(\lambda_j)e_j\otimes e_j + \int_0^\infty dk\, g(k^2)\Big[\tilde{e}_{-k}\otimes\tilde{e}_{-k} + \tilde{e}_k\otimes\tilde{e}_k\Big],$$

where

$$\tilde{e}_k = \Big(R(k)[\chi, \tfrac{d^2}{dx^2}] - \chi + 1\Big)e_k.$$

To derive Vodev's identity, write

$$R(k) - R(k') = (k^2 - (k')^2)R(k)R(k'),$$
$$1 = \chi(2-\chi) + (1-\chi)^2,$$
$$(1-\chi)R(k') = R_0(k')\Big(1 - \chi + [\tfrac{d^2}{dx^2}, \chi]R(k)\Big),$$

and deduce

$$R(k) - R(k') = \Big(k^2 - (k')^2\Big) R(k)\chi(2-\chi)R(k') + \Big\{R(k)[\chi, \tfrac{d^2}{dx^2}] - \chi + 1\Big\}(R_0(k) - R_0(k'))\Big\{1 - \chi + [\tfrac{d^2}{dx^2}, \chi]R(k)\Big\}$$

Vodev's identity also proves that if we let $\Omega \subset \mathbb{R}^d$ be an open set (or a Riemannian manifold) which agrees with $\mathbb{R}^d$ outside of a bounded region, and we define $A\colon \{u \in H_0^1(\Omega)\colon \operatorname{div}(\kappa \text{ grad } u) \in L^2(\Omega)\} \to L^2(\Omega)$ by

$$A = -\operatorname{div}(\kappa \text{ grad } u) + Vu,$$

where $\kappa = 1$ and $V = 0$ outside of a bounded region, then the spectrum of A consists of $[0, \infty)$ together with up to finitely many negative eigenvalues. If we allow V to be more general, for example a Coulomb potential, we get the same picture except near $\lambda = 0$, where we can now have an accumulation of eigenvalues.

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