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Boundary Values for an Eigenvalue Problem with a Singular Potential

ALLAN M. KRALL

*Department of Mathematics, McAllister Building,
The Pennsylvania State University, University Park, Pennsylvania 16802*

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The radial Hamiltonian operator $H = -d^2/dx^2 - \lambda/x^2$ is considered on $[0, \infty)$. While no boundary condition is needed at ∞ in order to make H self-adjoint, one is indeed needed at 0. This article describes in elementary terms how such conditions may be found. The resulting eigenvalue problem is then discussed and its relation to previous work is explained. Other potentials with singularities at 0 are also mentioned.

INTRODUCTION

In 1950 Case [3] discussed the boundary value problem generated by the Hamiltonian operator

$$H = -\frac{d^2}{dx^2} - \frac{\lambda}{x^2}, \quad \lambda > \frac{1}{4},$$

constrained by the boundary condition $\psi(0) = 0$, also requiring that solutions be in $L^2(0, \infty)$. Since he was only interested in eigenvalues and eigenfunctions, he only considered the equation

$$-\psi'' - \frac{\lambda}{x^2} \psi = \mu \psi,$$

with $\mu = -\tau^2 < 0$. He arrived at a formula for eigenvalues which contained an unexplained parameter B , undetermined since the boundary condition $\psi(0) = 0$ was inappropriate.

Case also discussed the problem generated by the Hamiltonian operator

$$H = -\frac{d^2}{dx^2} - \frac{\lambda}{x^n} + \frac{l(l+1)}{x^2}$$

with the same kind of result.

Realizing that the boundary value problem was not correctly formulated, Burnap *et al.* [2] followed an approach based on deficiency space theory, where the parameter determining the boundary condition at 0 is introduced through solutions of the equations $H\psi = \pm i\psi$. A formula for the (negative) eigenvalues was found, but the resulting description of the self-adjoint extensions generated by the minimal operator H_0 , associated with H , is difficult to understand, largely because, although they did not require $\psi(0) = 0$, they did not find a satisfactory substitute for it.

In both papers the possibility of spectrum in the range $\mu \geq 0$ was ignored because, as it turns out, there are no positive eigenvalues.

The problem had actually been "solved" earlier, however, by Meetz [13] in 1964, who found the negative eigenvalues as well as the formula for the spectral density function by using deficiency index theory and a formulation of limit circle boundary conditions at 0 based on solutions of the equation $H\psi = \pm i\psi$.

Further, Kodaira also considered the problem in [9]. Unfortunately when this work was republished in English, the problem in question was not included. Titchmarsh [16] and others [4, 11] have described what goes on theoretically, but a practical application of those results is not well known. References [4], [5], [11] and [16] do not provide much help in describing what such a constraint should be.

Recently, however, Fulton [6] has given a formulation of limit circle boundary conditions, which is applicable to an arbitrary limit circle end point, and makes use of limits of Wronskian combinations with a fixed pair of solutions for $\mu = 0$. The purpose of the present paper is to demonstrate the utility of Fulton's approach by applying it straightforwardly to obtain the negative eigenvalue formula, previously obtained by Meetz [13], Burnap *et al.* [2] and Kodaira [9], as well as the entire spectral resolution. The method employed represents a significant simplification over the methods used by the above authors, all of whom ran into considerable computational problems.

An interesting question arises as a result of Fulton's method: Are there any physical grounds for choosing the boundary value parameter introduced by the method?

The problem we ultimately define has a limit circle boundary condition at 0. The spectrum of the operator H_α thus generated consists of point spectrum (eigenvalues) when $\mu < 0$ and continuous spectrum when $\mu \geq 0$. The resulting spectral resolution of H_α strongly resembles the operator considered by Naimark [15]:

$$Ly = -y'' + qy,$$

where $\int_0^\infty e^{\epsilon x} |q(x)| dx < \infty$, subject to the constraint $y(0) - hy'(0) = 0$. It

contains a continuous integral in μ from 0 to ∞ , and then a sum due to isolated eigenvalues when $\mu < 0$.

SOLUTIONS

We consider the equation

$$-\frac{d^2\psi}{dx^2} - \frac{\lambda}{x^2}\psi = \mu\psi$$

in the interests of simplicity. Results for the other potentials, which are similar, are reserved for the last section.

Let us first consider solutions near 0. If $\mu = 0$, the differential equation is an Euler equation with two exact solutions given by

$$\psi_{10} = x^{1/2} \cos(\lambda' \ln x) / \sqrt{\lambda'}$$

and

$$\psi_{20} = x^{1/2} \sin(\lambda' \ln x) / \sqrt{\lambda'}$$

where $\lambda' = \sqrt{\lambda - \frac{1}{4}} > 0$. When $\mu \neq 0$, the method of Frobenius [8] shows that there exist two solutions $\psi_{1\mu}$ and $\psi_{2\mu}$ with behavior

$$\psi_{1\mu} = \psi_{10}(1 + O(1)),$$

$$\psi_{2\mu} = \psi_{20}(1 + O(1))$$

as x approaches 0. In each case both solutions are square integrable toward 0. The point $x = 0$ is in the "limit circle" case, and a boundary condition of some sort is required there in order to properly define a boundary value problem.

As x approaches ∞ , the approach is a bit different. Following Naimark [15], we let $\sqrt{\mu} = s = \sigma + i\tau$, $\tau \geq 0$. With a little "welding," we find there are two linearly independent solutions ψ_1 and ψ_2 which are continuous for $x \geq 0$, $\tau \geq 0$ and which are holomorphic in s when $\tau > 0$. They have the asymptotic properties

$$\psi_1(x, s) = e^{isx}(1 + O(1)),$$

$$\psi_1'(x, s) = e^{isx}(is + O(1)),$$

$$\psi_2(x, s) = e^{-isx}(1 + O(1)),$$

$$\psi_2'(x, s) = e^{-isx}(-is + O(1))$$

uniformly as x approaches ∞ . $W[\psi_1, \psi_2] = -2is$. As s approaches ∞ ,

$$\begin{aligned} \psi_1(x, s) &= e^{isx}(1 + O(1/s)), \\ \psi_1'(x, s) &= ise^{isx}(1 + O(1/s)), \\ \psi_2(x, s) &= e^{-isx}(1 + O(1/s)), \\ \psi_2'(x, s) &= -ise^{-isx}(1 + O(1/s)). \end{aligned}$$

For $\tau > 0$ only ψ_1 is square integrable toward ∞ . The point ∞ is in the limit point case, and no boundary conditions is required there is order to properly defined a boundary value problem.

We note in passing that when $s = i\tau$, $\psi_1(x, i\tau) = \sqrt{2/\pi} x^{1/2} K_{i\lambda}(\tau x)$ (see [14, p. 1323]).

GREEN'S FORMULA, BOUNDARY CONDITIONS

We denote by D those elements f which satisfy the following.

- (a) f is in $L^2(0, \infty)$.
- (b) f' exists and is absolutely continuous on every finite subinterval of $[0, \infty)$.
- (c) Hf is in $L^2(0, \infty)$.

Then an elementary computation shows that for f, g in D

$$\int_0^\infty [(Hf)\bar{g} - f(\overline{Hg})] dx = W[f, \bar{g}]_0^\infty.$$

The integral is finite, so the limits on the right exist. Further, since the limit point case holds at ∞ , the limit at ∞ is 0:

$$\int_0^\infty [(Hf)\bar{g} - f(\overline{Hg})] dx = -\lim_{x \rightarrow 0} W[f, \bar{g}].$$

Note that the limit on the right is finite, although it is not necessarily 0, for all f, g in D . It is in the proper exploitation of this expression that is the key to all that follows. We note in particular that for $\mu = s = 0$, $\lim_{x \rightarrow 0} W[f, \psi_{10}]$ and $\lim_{x \rightarrow 0} W[f, \psi_{20}]$ exist and are finite. These are the building blocks in the expansion of $W[f, \bar{g}]$.

Let α be any number $0 \leq \alpha \leq 2\pi$. Then define

$$\begin{aligned} B_1(f) &= \lim_{x \rightarrow 0} W[f, \psi_{1\alpha}], \\ B_2(f) &= \lim_{x \rightarrow 0} W[f, \psi_{2\alpha}], \end{aligned}$$

and

$$\begin{aligned} A(f) &= B_1(f) \sin \alpha + B_2(f) \cos \alpha, \\ B(f) &= -B_2(f) \sin \alpha + B_1(f) \cos \alpha. \end{aligned}$$

THEOREM. *Let f, g be in D . Then*

$$\int_0^\infty [(Hf)\bar{g} - f\overline{(Hg)}] dx = A(f)\overline{B(g)} - B(f)\overline{A(g)}.$$

Proof.

$$\begin{aligned} -\lim_{x \rightarrow 0} W[f, \bar{g}] &= \lim_{x \rightarrow 0} (W[f\bar{g}])(-W[\psi_{10}, \psi_{20}]) \\ &= \lim_{x \rightarrow 0} \begin{vmatrix} f & f' \\ \bar{g} & \bar{g}' \end{vmatrix} \begin{vmatrix} \psi'_{20} & \psi'_{10} \\ -\psi_{20} & -\psi_{10} \end{vmatrix} \begin{vmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{vmatrix} \\ &= \lim_{x \rightarrow 0} \left| \begin{pmatrix} f & f' \\ \bar{g} & \bar{g}' \end{pmatrix} \begin{pmatrix} \psi'_{20} & \psi'_{10} \\ -\psi_{20} & -\psi_{10} \end{pmatrix} \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \right| \\ &= \lim_{x \rightarrow 0} \left| \begin{pmatrix} f\psi'_{20} - f'\psi_{20} & f\psi'_{10} - f'\psi_{10} \\ \bar{g}\psi'_{20} - \bar{g}'\psi_{20} & \bar{g}\psi'_{10} - \bar{g}'\psi_{10} \end{pmatrix} \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \right| \\ &= \begin{vmatrix} B_2(f) \cos \alpha + B_1(f) \sin \alpha & -B_2(f) \sin \alpha + B_1(f) \cos \alpha \\ B_2(\bar{g}) \cos \alpha + B_1(\bar{g}) \sin \alpha & -B_2(\bar{g}) \sin \alpha + B_1(\bar{g}) \cos \alpha \end{vmatrix} \\ &= \begin{vmatrix} A(f) & B(f) \\ A(\bar{g}) & B(\bar{g}) \end{vmatrix} \\ &= A(f)\overline{B(g)} - B(f)\overline{A(g)}. \end{aligned}$$

We note that each of these expressions is finite separately. By appropriately choosing α , $A(f)$ can generate an arbitrary boundary condition at 0. $B(g)$ is the complementary boundary condition [4].

We denote by D_α those elements of which satisfy the following.

- (a) f is in D .
- (b) $A(f) = 0$.

For f in D_α we define H_α by setting $H_\alpha f = Hf$.

THEOREM. H_α is self-adjoint.

Proof. It is apparent that D_α is dense in $L^2(0, \infty)$ (see [15, p. 105]), so H_α^* exists.

Let f be in $D_\alpha \cap C_{00}(0, \infty)$, and suppose that $f \equiv 0$ when $0 \leq x < a$. Then for g in the domain of H_α^* ,

$$(H_\alpha f, g) = (f, H_\alpha^* g),$$

where (\cdot, \cdot) denotes the inner product in $L^2(0, \infty)$. This is the same as

$$\int_0^\infty \left(-f'' - \frac{\lambda}{x^2} f\right) \bar{g} \, dx = \int_0^\infty f \overline{(H_\alpha^* g)} \, dx.$$

Putting the terms with f together and integrating by parts twice yields

$$\int_0^\infty f'' \left[g + \int_a^x \int_a^y (\lambda g/z^2 + (H_\alpha^* g)) \, dz \, dy \right]^* \, dx = 0.$$

Since such f'' 's are dense in $L^2(0, \infty)$,

$$g + \int_a^x \int_a^y (\lambda g/z^2 + (H_\alpha^* g)) \, dz \, dy = 0.$$

Two differentiations then reveal that

$$H_\alpha^* g = -g'' - \frac{\lambda}{x^2} g.$$

Thus H_α^* has the same form as H_α .

If, now, f is any element in D_α , then Green's formula shows

$$\begin{aligned} 0 &= (H_\alpha f, g) - (f, H_\alpha^* g) \\ &= A(f) \overline{B(g)} - \overline{B(f)} A(g) \\ &= -\overline{B(f)} A(g), \end{aligned}$$

since $A(f) = 0$. Further, since $B(f)$ is arbitrary, $A(g) = 0$ as well. Hence the domain of H_α^* is in D_α . The converse inclusion is trivial, and so H_α is self-adjoint.

THE SPECTRUM OF H_α

When $\mu > 0$ the asymptotic formulas show that $|\psi_1|^2$ and $|\psi_2|^2$ both approach 1 as x approaches ∞ , so neither can be an eigenfunction. Likewise, Naimark [15, p. 126] shows that no linear combination can be square integrable either, so there are no eigenvalues on the positive μ axis.

On the other hand Naimark's arguments [15, p. 135] show that the

positive μ axis is contained in the spectrum since the resolvent is only densely defined.

THEOREM. *Each point of the positive μ axis, $\mu \geq 0$, is in the continuous spectrum of H_α .*

Proof. Since H_α is self-adjoint $\sigma(H_\alpha) = \sigma_p(H_\alpha) \cup \sigma_c(H_\alpha)$. When $\mu = -\tau^2 < 0$, however, there is a solution (see [14; p. 1323])

$$\psi_1(x, i\tau) = \sqrt{2/\pi} x^{1/2} K_{i\lambda'}(\tau x),$$

which is square integrable toward ∞ , and, thus, is an eigenfunction (with eigenvalue $-\tau^2$) provided $A(\psi_1) = 0$. In order to see when that occurs some approximating is necessary.

In

$$\psi'' + \frac{\lambda'^2 + \frac{1}{4}}{x^2} \psi = \tau^2 \psi,$$

set $\psi = x^{1/2}y$ and $\tau x = t$ to find that y satisfies

$$t^2 \frac{d^2 y}{dt^2} + t \frac{dy}{dt} - (t^2 - \lambda'^2)y = 0.$$

The solution we seek is

$$y = K_{i\lambda'}(t) = \frac{\pi}{2 \sin i\lambda' \pi} (I_{-i\lambda'}(t) - I_{i\lambda'}(t)),$$

where (see [1])

$$I_\nu(t) = \sum_{m=0}^{\infty} \frac{(t/2)^{\nu+2m}}{m! \Gamma(m+\nu+1)}.$$

Near $t = 0$, $I_\nu(t) \approx (t/2)^\nu / \Gamma(\nu+1)$, so

$$K_{i\lambda'}(\tau x) \approx \frac{\pi}{2 \sin i\lambda' \pi} \left[\frac{(\tau x/2)^{-i\lambda'}}{\Gamma(-i\lambda'+1)} - \frac{(\tau x/2)^{i\lambda'}}{\Gamma(i\lambda'+1)} \right],$$

and so ψ_1 satisfies near $x = 0$,

$$\psi_1(x, i\tau) \approx \frac{\pi x^{1/2}}{2 \sin i\lambda' \pi} \left[\frac{(\tau x/2)^{-i\lambda'}}{\Gamma(-i\lambda'+1)} - \frac{(\tau x/2)^{i\lambda'}}{\Gamma(i\lambda'+1)} \right].$$

Now if $\mu = 0$, there are two solutions

$$\begin{aligned}\psi_+(x) &= x^{1/2} x^{i\lambda'}, \\ \psi_-(x) &= x^{1/2} x^{-i\lambda'}\end{aligned}$$

to $\psi'' + (\lambda'^2 + \frac{1}{4})/x^2 \psi = 0$. Therefore $\psi_{10} = [\psi_+ + \psi_-]/2\sqrt{\lambda'}$ and $\psi_{20} = [\psi_+ - \psi_-]/2i\sqrt{\lambda'}$. In order for ψ_1 to be an eigenfunction, ψ_1 must be proportional to $\sin \alpha \psi_{10} + \cos \alpha \psi_{20}$ in order to satisfy $A(\psi_1) = 0$. That is,

$$\begin{aligned}\psi_1 &\approx \frac{-i\psi_+}{2\sqrt{\lambda'}} e^{i\alpha} + \frac{i\psi_-}{2\sqrt{\lambda'}} e^{-i\alpha} \\ &\approx \frac{ix^{1/2}}{2\sqrt{\lambda}} (-x^{i\lambda'} e^{i\alpha} + x^{-i\lambda'} e^{-i\alpha}).\end{aligned}$$

Matching coefficients between these two expressions for ψ_1 we find

$$e^{i\alpha} A = \frac{(\tau/2)^{i\lambda'}}{\Gamma(i\lambda' + 1)},$$

where A is real. Taking arguments and solving for τ , we find

$$\tau = 2 \exp[(\alpha + \arg \Gamma(i\lambda' + 1))/\lambda'] \exp(k\pi/\lambda'),$$

where k is an integer. This formula reestablishes formulas 25 of [2] as well as making precise the results of [3].

THEOREM. *The negative μ axis, $\mu < 0$, contains only isolated eigenvalues $\mu = -\tau^2$, where τ is given by*

$$\tau = 2 \exp[(\alpha + \arg \Gamma(i\lambda' + 1))/\lambda'] \exp(k\pi/\lambda'),$$

$k = 0, \pm 1, \pm 2, \dots$, with corresponding eigenfunction $\sqrt{2/\pi} x^{1/2} K_{i\lambda'}(\tau x)$. The eigenvalues $\mu = -\tau^2$ have points of accumulation only at 0 and $-\infty$. Other values of $\mu < 0$ are in the resolvent of H_α .

THE SPECIAL RESOLUTION OF H_α

There are at least two approaches to deriving the spectral resolution of H_α . Titchmarsh [16] uses contour integration, while Coddington and Levinson [4] achieve the same results via the Helley selection theorems. Since this ground has been well worked over, we illustrate only the high spots.

The Green's function of H_α is given by $G(s_0^2, x, \xi) = G_1(s_0^2, x, \xi) + G_2(s_0^2, x, \xi)$, where

$$\begin{aligned} G_1(s_0^2, x, \xi) &= -\frac{1}{2is_0} \psi_1(\xi, s_0) \psi_2(x, s_0), & \xi > x, \\ &= -\frac{1}{2is_0} \psi_1(x, s_0) \psi_2(\xi, s_0), & x > \xi, \end{aligned}$$

and

$$G_2(s_0^2, x, \xi) = \frac{1}{2is_0} \frac{A(\psi_2(x, s_0))}{A(\psi_1(x, s_0))} \psi_1(x, s_0) \psi_1(\xi, s_0)$$

whenever $\mu = s_0^2$ is not in the spectrum of H_α . The resolvent of H_α is then given by

$$\psi(x) = \int_0^\infty G(s_0^2, x, \xi) f(\xi) d\xi.$$

That is, ψ satisfies $(H_\alpha - \mu)\psi = f$.

Through contour integration [11, 15, 16], $G(s_0^2, x, \xi)$ can be expanded to yield

THEOREM.

$$\begin{aligned} G(s_0^2, x, \xi) &= \sum_k \frac{\psi_1(x, s_k) \psi_1(\xi, s_k)}{(s_k^2 - s_0^2) \int_0^\infty \psi_1(\xi, s_k)^2 d\xi} \\ &\quad - \frac{1}{2\pi} \int_0^\infty \frac{\tilde{\psi}(x, s) \tilde{\psi}(\xi, s) ds}{(s^2 - s_0^2) A(\psi_1) A(\psi_2)}, \end{aligned}$$

where $(s_k)^2 = (i\tau_k)^2 = \mu_k^2$ are the eigenvalues of H_α and $\tilde{\psi}(x, s) = A(\psi_2) \psi_1(x, s) - A(\psi_1) \psi_2(x, s)$.

We note that if $A(\psi_1) = 0$ on the real s axis, then $A(\psi_2) = 0$ as well, since they are complex conjugates. At such points $\tilde{\psi}$ also vanishes and so these "singularities" of G are removable.

This expansion of the Green's function then paves the way for the expansion of elements in $L^2(0, \infty)$:

THEOREM.

$$\begin{aligned} f(x) &= \sum_k \alpha_k \psi_1(x, s_k) \left/ \left(\int_0^\infty \psi_1(\xi, s_k)^2 d\xi \right)^{1/2} \right. \\ &\quad \left. - \frac{1}{2\pi} \int_0^\infty \alpha(s) (\tilde{\psi}(x, s) / |A(\psi_1)|) ds, \right. \end{aligned}$$

where

$$\alpha_k = \int_0^\infty f(\xi) \psi_1(\xi, s_k) d\xi \left/ \left(\int_0^\infty \psi_1(\xi, s_k)^2 d\xi \right)^{1/2} \right.$$

$$\alpha(s) = \int_0^\infty f(\xi) (\tilde{\psi}(\xi, s) / |A(\psi_1)|) ds.$$

Convergence is valid in the mean sense if f is in $L^2(0, \infty)$ [4], in the pointwise sense under stronger conditions on f [15].

OTHER POTENTIALS

The results for

A. $H\psi = -\frac{d^2\psi}{dx^2} - \frac{\lambda}{x^n} \psi,$

B. $H\psi = -\frac{d^2\psi}{dx^2} - \frac{\lambda\psi}{x^4} + \frac{l(l+1)}{x^2}$

are virtually unchanged in form from those just presented. Example A, discussed by Case [3], is in the limit circle case at 0 with solutions to $H\psi = 0$ given by

$$x^{n/4} \cos \left(\frac{2}{n-2} \left(\frac{\lambda}{x^{n-2}} \right)^{1/2} \right) \quad \text{and} \quad x^{n/4} \sin \left(\frac{2}{n-2} \left(\frac{\lambda}{x^{n-2}} \right)^{1/2} \right).$$

Example B, discussed in [2], is algebraically more of a nuisance, but is also in the limit circle case at 0 with solutions near zero given in terms of Hankel functions [12, 17].

Remarks. Another form of the spectral resolution can be obtained by following a Titchmarsh-type approach recently given by Fulton [7]. By using solutions θ, ϕ of $H\psi = \mu\psi, \mu$ complex, satisfying

$$\begin{pmatrix} B_1(\theta) \\ B_2(\theta) \end{pmatrix} = \begin{pmatrix} \sin \alpha \\ \cos \alpha \end{pmatrix}, \quad \begin{pmatrix} B_1(\phi) \\ B_2(\phi) \end{pmatrix} = \begin{pmatrix} \cos \alpha \\ -\sin \alpha \end{pmatrix},$$

and defining $m(\mu)$ be requiring $\theta + m\phi$ to be in $L^2(0, \infty)$, the spectral measure ρ can be found by setting

$$\rho(\mu) = \lim_{\epsilon \searrow 0} \frac{1}{\pi} \int_0^\mu -\text{Im } m(\mu + i\epsilon) d\mu.$$

This gives a result equivalent to that of Meetz [13], although considerable labor is required to make the connection.

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