Spectral Functions for Regular Sturm-Liouville Problems

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Regular One-dimensional Sturm-Liouville Problems

Let $I = [0, 1] \subset \mathbb{R}$, and let $\mathcal{L}$ be the following symmetric second order differential operator

$$\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + V(x) \ ,$$

with $p(x) > 0$ for $x \in I$, and $p(x)$ and $V(x)$ in $\mathscr{L}^1(I, \mathbb{R})$. For the differential operator $\mathcal{L}$ we consider the differential equation

$$\mathcal{L}\varphi_\lambda = \lambda^2\varphi_\lambda \ , \tag{1}$$

where $\lambda \in \mathbb{C}$ and $\varphi_\lambda \in C^2(I)$.
The differential equation (1) endowed with self-adjoint boundary conditions imposed on φ_λ is called a regular *Sturm-Liouville* problem. Furthermore, the parameter $\lambda \in \mathbb{R}$ denotes the eigenvalues of the SL problem.
Self-adjoint boundary conditions can be divided in two mutually excluding classes:

- *Separated* Boundary Conditions
- *Coupled* boundary conditions.

Separated Boundary Conditions

Separated boundary conditions have the following general form

$$\begin{aligned} A_1\varphi_\lambda(0) - A_2 p(0)\varphi'_\lambda(0) &= 0 \ , \\ B_1\varphi_\lambda(1) + B_2 p(1)\varphi'_\lambda(1) &= 0 \ , \end{aligned}$$

with $A_1, A_2, B_1, B_2 \in \mathbb{R}$ and $(A_1, A_2) \neq (0, 0)$, and $(B_1, B_2) \neq (0, 0)$.
Eigenvalues. For each λ we choose a solution φ_λ satisfying the *initial conditions*

$$\varphi_\lambda(0) = A_2 \ , \quad \text{and} \quad p(0)\varphi'_\lambda(0) = A_1 \ .$$

The eigenfunctions of the Sturm-Liouville problem are, then, those that also satisfy the condition

$$\Omega(\lambda) = B_1\varphi_\lambda(1) + B_2 p(1)\varphi'_\lambda(1) = 0 \ ,$$

which represents an *implicit* equation for the eigenvalues λ.
Remarks: Well-known examples

- For $A_1 = B_1 = 0$ and $A_2 = B_2 = 0$ we get Neuman and Dirichlet boundary conditions, respectively.
- When $A_1 = B_1$ and $A_2 = -B_2$ we have Robin Boundary conditions.
- By setting $A_1 = B_2 = 0$ or $A_2 = B_1 = 0$ we obtain mixed or hybrid boundary conditions.

Coupled Boundary Conditions

Coupled boundary conditions can be expressed in general as

$$\begin{pmatrix} \varphi_\lambda(1) \\ p(1)\varphi'_\lambda(1) \end{pmatrix} = e^{i\gamma}\mathrm{K} \begin{pmatrix} \varphi_\lambda(0) \\ p(0)\varphi'_\lambda(0) \end{pmatrix} ,$$

where $-\pi < \gamma \leq 0$ or $0 \leq \gamma < \pi$ and $\mathrm{K} \in \mathrm{SL}_2(\mathbb{R})$. For $\gamma = 0$ and $\mathrm{K} = I_2$ we have periodic boundary conditions.

Eigenvalues. We write the solution as

$$\varphi_\lambda(x) = \alpha u_\lambda(x) + \beta v_\lambda(x) ,$$

where for each λ, $u_\lambda(x)$ and $v_\lambda(x)$ are defined by the initial conditions

$$\varphi_\lambda(0) = \beta \quad \text{and} \quad p(0)\varphi'_\lambda(0) = \alpha .$$

By imposing coupled boundary conditions and by denoting $[k_{ij}] = K$ we obtain the linear system

$$\begin{aligned} \alpha\left[u_\lambda(1) - e^{i\gamma}k_{12}\right] + \beta\left[v_\lambda(1) - e^{i\gamma}k_{11}\right] &= 0 \\ \alpha\left[p(1)u'_\lambda(1) - e^{i\gamma}k_{22}\right] + \beta\left[p(1)v'_\lambda(1) - e^{i\gamma}k_{21}\right] &= 0 , \end{aligned}$$

which has a non-trivial solution if and only if

$$\Delta(\lambda) = 2\cos\gamma - \left[k_{22}v_\lambda(1) - k_{12}u_\lambda(1) + k_{11}p(1)u'_\lambda(1) - k_{12}p(1)v'_\lambda(1)\right] = 0 .$$

Spectral Zeta Function

The implicit equations for the eigenvalues provide an integral representation of the spectral zeta function valid for $\Re(s) > 1/2$ as

$$\zeta^{\left\{ \substack{\mathrm{S} \\ \mathrm{C}} \right\}}(s) = \frac{1}{2\pi i} \int_{\mathcal{C}^{\left\{ \substack{\mathrm{S} \\ \mathrm{C}} \right\}}} \mathrm{d}\lambda \lambda^{-2s} \frac{\partial}{\partial \lambda} \ln \left\{ \begin{array}{c} \Omega(\lambda) \\ \Delta(\lambda) \end{array} \right\} .$$

By deforming the contour to the imaginary axis and by changing variables $i\lambda \to z$ one obtains the representation

$$\zeta^{\left\{ \substack{\mathrm{S} \\ \mathrm{C}} \right\}}(s) = \frac{\sin \pi s}{\pi} \int_0^\infty \mathrm{d}z z^{-2s} \frac{\partial}{\partial z} \ln \left\{ \begin{array}{c} \Omega(z) \\ \Delta(z) \end{array} \right\} ,$$

valid for $1/2 < \Re(s) < 1$.

To perform the analytic continuation to the left of the strip $1/2 < \Re(s) < 1$ we subtract and add from the integrand a suitable number of terms from the asymptotic expansion of $\ln \Omega(z)$ and $\ln \Delta(z)$ for $z \to \infty$.

The desired asymptotic expansion is obtained through a *WKB analysis of the solutions of Sturm-Liouville problem.*

Remark:

- For a general one-dimensional Sturm-Liouville differential operator with general self-adjoint boundary conditions, $\Omega(z)$ and $\Delta(z)$ are *not known* explicitly.

WKB Expansion

In the parameter z, the Sturm-Liouville differential equation reads

$$\left[-\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right)+V(x)\right]\varphi_z(x) = -z^2\varphi_z(x) \ .$$

By introducing the auxiliary function

$$\mathcal{S}(x,z) = \frac{\partial}{\partial x}\ln\varphi_z(x) \ ,$$

the equation above is equivalent to the following

$$[p(x)\mathcal{S}(x,z)]' = V(x) + z^2 - p(x)\mathcal{S}^2(x,z) \ .$$

As $z \to \infty$ we assume that $\mathcal{S}(x,z)$ has the asymptotic expansion

$$\mathcal{S}(x,z) \sim zS_{-1}(x) + S_0(x) + \sum_{i=1}^{\infty}\frac{S_i(x)}{z^i} \ .$$

Once the asymptotic expansion of $\mathcal{S}(x,z)$ is known, the one for the solution $\varphi_z(x)$ will *immediately* follow.

WKB Expansion

By substituting the asymptotic form of $\mathcal{S}(x,z)$ in the previous non-linear differential equation we obtain

$$S_{-1}^{\pm}(x) = \pm\frac{1}{\sqrt{p(x)}}\,, \qquad S_0^{\pm}(x) = -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\ln\left(p(x)S_{-1}^{\pm}(x)\right) = -\frac{p'(x)}{4p(x)}\,,$$

$$S_1^{\pm}(x) = \frac{1}{2p(x)S_{-1}^{\pm}(x)}\left[V(x) - p(x)\left(S_0^{\pm}\right)^2(x) - \left(p(x)S_0^{\pm}(x)\right)'\right]\,,$$

and for $i \geq 1$

$$S_{i+1}^{\pm}(x) = -\frac{1}{2p(x)S_{-1}^{\pm}(x)}\left[\left(p(x)S_i^{\pm}(x)\right)' + p(x)\sum_{m=0}^{i} S_m^{\pm}(x)S_{i-m}^{\pm}(x)\right]\,.$$

The terms $S_i^{+}(x)$ and $S_i^{-}(x)$ provide the exponentially growing and decaying parts of the solution $\varphi_z(x)$ as

$$\varphi_z(x) = A\exp\left\{\int_0^x \mathcal{S}^{+}(t,z)\mathrm{d}t\right\} + B\exp\left\{\int_0^x \mathcal{S}^{-}(t,z)\mathrm{d}t\right\}\,,$$

with A and B uniquely determined by the *initial* conditions.

Asymptotic Expansion: Separated Boundary Conditions

For separated boundary conditions the implicit equation for the eigenvalues is

$$\begin{aligned}\ln\Omega(z) &\sim \ln\left[-A_2 p(0)\mathcal{S}^-(0,z)+A_1\right]+\ln\left[B_2 p(1)\mathcal{S}^+(1,z)+B_1\right]\\ &- \ln\left[p(0)\left(\mathcal{S}^+(0,z)-\mathcal{S}^-(0,z)\right)\right]+\int_0^1 \mathcal{S}^+(t,z)\mathrm{d}t\,.\end{aligned}$$

By introducing the function $\delta(x)=1$ for $x=0$, and $\delta(x)=0$ for $x\neq 0$ one can further expand $\ln\Omega(z)$ to obtain

$$\begin{aligned}\ln\Omega(z) &= -\frac{1}{4}\ln p(0)p(1)+[1-\delta(A_2)]\ln A_2\sqrt{p(0)}+[1-\delta(B_2)]\ln B_2\sqrt{p(1)}\\ &+ \delta(A_2)\ln A_1+\delta(B_2)\ln B_1-\ln 2z+[2-\delta(A_2)-\delta(B_2)]\ln z\\ &+ z\int_0^1 S^+_{-1}(t)\mathrm{d}t+\sum_{i=1}^{\infty}\frac{\mathcal{M}_i}{z^i}\,.\end{aligned}$$

Remark:

- The terms $\mathcal{M}_i$, $i\geq 1$, are expressed *only* in terms of $p^{(n)}(x)$ and $V^{(n)}(x)$ with $n\leq i+1$ and their powers.

Asymptotic Expansion: Coupled Boundary Conditions

For coupled boundary conditions the implicit equation for the eigenvalues is

$$\ln\Delta(z) \sim -\ln\left[p(0)\left(\mathcal{S}^+(0,z)-\mathcal{S}^-(0,z)\right)\right] + \int_0^1 \mathcal{S}^+(t,z)\mathrm{d}t$$
$$+\ln\left[-k_{21}-k_{22}p(0)\mathcal{S}^-(0,z)+k_{11}p(1)\mathcal{S}^+(1,z)+k_{12}p(1)p(0)\mathcal{S}^-(0,z)\mathcal{S}^+(1,z)\right]$$

The large-z asymptotic behavior depends on whether k_{12} vanishes or not. Both cases are described by the expression

$$\begin{aligned}\ln\Delta(z) &= -\frac{1}{4}\ln p(0)p(1) + [1-\delta(k_{12})]\ln k_{12}\sqrt{p(0)p(1)} \\ &+ \delta(k_{12})\ln\left(k_{22}\sqrt{p(0)}+k_{11}\sqrt{p(1)}\right) \\ &+ [2-\delta(k_{12})]\ln z - \ln 2z + z\int_0^1 S_{-1}^+(t)\mathrm{d}t + \sum_{i=1}^{\infty}\frac{\mathcal{N}_i}{z^i}\ .\end{aligned}$$

Remark:

- The terms $\mathcal{N}_i$, $i \geq 1$, are expressed *only* in terms of $p^{(n)}(x)$ and $V^{(n)}(x)$ with $n \leq i+1$ and their powers.

From the integral representation of $\zeta^{\left\{ \substack{\mathrm{S} \\ \mathrm{C}} \right\}}(s)$ we add and subtract L leading terms of the respective asymptotic expansions to obtain

$$\zeta^{\left\{ \substack{\mathrm{S} \\ \mathrm{C}} \right\}}(s) = Z^{\left\{ \substack{\mathrm{S} \\ \mathrm{C}} \right\}}(s) + \sum_{i=-1}^{L} A_i^{\left\{ \substack{\mathrm{S} \\ \mathrm{C}} \right\}}(s) \,,$$

with $Z^{\left\{ \substack{\mathrm{S} \\ \mathrm{C}} \right\}}(s)$ an analytic function for $\Re s > -(L+1)/2$, and $A_i^{\left\{ \substack{\mathrm{S} \\ \mathrm{C}} \right\}}(s)$ meromorphic functions for $s \in \mathbb{C}$. In particular we have

$$\zeta^{\mathrm{S}}(s) = Z^{\mathrm{S}}(s) + \frac{\sin \pi s}{\pi} \left[\frac{1 - \delta(A_2) - \delta(B_2)}{2s} + \frac{1}{2s-1} \int_0^1 S_{-1}^{+}(t) \mathrm{d}t - \sum_{i=1}^{L} i \frac{\mathcal{M}_i}{2s+i} \right] \,,$$

$$\zeta^{\mathrm{C}}(s) = Z^{\mathrm{C}}(s) + \frac{\sin \pi s}{\pi} \left[\frac{1 - \delta(k_{12})}{2s} + \frac{1}{2s-1} \int_0^1 S_{-1}^{+}(t) \mathrm{d}t - \sum_{i=1}^{L} i \frac{\mathcal{N}_i}{2s+i} \right] \,.$$

Remarks:

- $\zeta^{\mathrm{S}}(s)$ and $\zeta^{\mathrm{C}}(s)$ are meromorphic functions of $s \in \mathbb{C}$ with only a simple pole at $s = 1/2$.

Functional Determinant and Heat Kernel Coefficients

From the analytically continued expression of the spectral zeta function one can compute

- The functional determinant, $\det(\mathcal{L}) = \exp\{-\zeta'(0)\}$.
- The coefficients of the asymptotic expansion of $\theta(t) = \mathrm{Tr}_{\mathscr{L}^2} e^{-t\mathcal{L}}$.

For the HKC, by using the Mellin transform one has

$$a_{\frac{1}{2}-s} = \Gamma(s)\mathrm{Res}\,\zeta(s)\;, \quad a_{\frac{1}{2}+n} = \frac{(-1)^n}{n!}\zeta(-n)\;.$$

when $s = 1/2$ and $s = -(2n+1)/2$ with $n \in \mathbb{N}_0$. In our case we have

$$a_0^{\mathrm{S}} = a_0^{\mathrm{C}} = \frac{1}{2\sqrt{\pi}} \int_0^1 \frac{\mathrm{d}t}{\sqrt{p(t)}}\;,$$

$$a_{\frac{1}{2}}^{\mathrm{S}} = \frac{1-\delta(A_2)-\delta(B_2)}{2}\;,\; a_{\frac{2m+1}{2}}^{\mathrm{S}} = -\frac{1}{(m-1)!}\mathcal{M}_{2m}\;,\; a_{n+1}^{\mathrm{S}} = -\frac{2^{2n}n!}{\sqrt{\pi}(2n)!}\mathcal{M}_{2n+1}\;,$$

$$a_{\frac{1}{2}}^{\mathrm{C}} = \frac{1-\delta(k_{12})}{2}\;, \quad a_{\frac{2m+1}{2}}^{\mathrm{C}} = -\frac{1}{(m-1)!}\mathcal{N}_{2m}\;, \quad a_{n+1}^{\mathrm{C}} = -\frac{2^{2n}n!}{\sqrt{\pi}(2n)!}\mathcal{N}_{2n+1}\;,$$

with $m \in \mathbb{N}^+$ and $n \in \mathbb{N}_0$.

Further Research

The analysis outlined above represents the foundation for further research

- Analysis of the Casimir energy and force for a one-dimensional piston modeled by a compact potential with separated or coupled boundary conditions. Study of the behavior of the force as the boundary conditions change.
- Generalize the technique presented here to study spectral functions for Laplace operator on manifolds of the type $I \times N$ or $I \times_f N$ with N being a compact Riemannian manifold, and $I = [a, b] \subset \mathbb{R}$. These results could be applied to the analysis of the Casimir effect for potential pistons with arbitrary cross-section.
- It would be particularly interesting to develop a method similar to the one presented in this paper to obtain the analytic continuation of the spectral zeta function for one-dimensional *singular* Sturm-Liouville problems:
  - The functions $p(x)$ and $V(x)$ become *unbounded* in the neighborhood of the endpoints of I.
  - The interval $I = \mathbb{R}$ is unbounded and the potential $V(x) \to +\infty$, as $|x| \to \infty$, is confining.