ANTON ZETTL

SELF-ADJOINT BOUNDARY CONDITIONS

ABSTRACT. A brief overview of the theory of self-adjoint ordinary differential operators in Hilbert space is given and the recently developed theory of symmetric differential expressions and boundary conditions which determine these operators is discussed. A short account of the recent solution of the deficiency index problem is provided.

1. INTRODUCTION

John von Neumann

" ... when America's National Academy of Science asked shortly before his death what he thought were his three greatest achievements ... Johnny replied to the academy that he considered his most important contributions to have been on the theory of self-adjoint operators in Hilbert space, and on the mathematical foundations of quantum theory and the ergotic theorem."

Macrae's biography of John von Neumann.

Applications

"From the point of view of applications, the most important single class of operators are the differential operators. The study of these operators is complicated by the fact that they are necessarily unbounded. Consequently, the problem of choosing a domain for a differential operator is by no means trivial; ... for unbounded operators the choice of domains can be quite crucial".

Dunford Schwartz v.II

A self-adjoint ordinary differential operator in Hilbert space is generated by two things:

(1) *A Symmetric Differential Expression.*
(2) *A Boundary Condition.*

Given such a self-adjoint differential operator, a basic question is: What is its spectrum ?

2. THE STURM-LIOUVILLE CASE

Consider the Sturm-Liouville equation

$$My = -(py')' + qy = \lambda wy, \ \lambda \in \mathbb{C}, \ J = (a,b), \ -\infty \le a < b \le +\infty, \tag{2.1}$$

with coefficient functions p, q and weight function w satisfying

$$\frac{1}{p}, \ q, \ w \in L^1(J,\mathbb{R}), \ p > 0, \ w > 0, \ a.e. \, on \ J, \tag{2.2}$$

and regular endpoints a and b. Let $M_n(\mathbb{X})$, $n \in \mathbb{N} = \{1, 2, 3, ...\}$ denote the set of n by n matrices with entries from the set $\mathbb{X}$ and consider the boundary condition

$$AY(a) + BY(b) = 0,\ A,\ B \in M_2(\mathbb{C}),\ Y = \begin{bmatrix} y \\ (py') \end{bmatrix}. \tag{2.3}$$

Then the self-adjoint operator realizations S of problem (2.1)-(2.3) satisfy

$$S_{\min} \subset S = S^* \subset S_{\max}, \tag{2.4}$$

where $S_{\min}$ denotes the minimal operator with domain $D_{\min}$ and $S_{\max}$ denotes the maximal operator with domain $D_{\max}$ in the Hilbert space $H = L^2(J, w)$. Note that the domains $D(S)$ of S is characterized by boundary conditions (2.3) with matrices $A,\ B$ satisfying

$$rank(A : B) = 2,\ AE_2A^* = BE_2B^*,\ E_2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}. \tag{2.5}$$

The linear manifold

$$D(S) = \{y \in D_{\max} : (2.3)\ \textit{and}\ (2.5)\ \textit{hold}\ \} \tag{2.6}$$

is the domain of a self-adjoint operator S and every operator S satisfying (2.4) is characterized this way.

It is well known that the self-adjoint boundary conditions (2.3) satisfying (2.5) can be classified into two mutually exclusive classes: coupled and separated, and these classes have the following canonical representations:

$$(A : B) = (e^{\mathrm{i}\gamma} K : I_2),\ \mathrm{i} = \sqrt{-1},\ -\pi < \gamma \le \pi, \tag{2.7}$$

with $I_k,\ k = 2, 3, \ldots$ denoting the k by k identity matrix and

$$K \in M_2(\mathbb{R}),\ \det(K) = 1;$$

and

$$\begin{aligned} \cos(\alpha)\, y(a) - \sin(\alpha)\, (py')(a) = 0,\ \alpha \in [0, \pi), \\ \cos(\beta)\, y(b) - \sin(\beta)\, (py')(b) = 0,\ \beta \in (0, \pi]; \end{aligned} \tag{2.8}$$

respectively. These are canonical forms of regular self-adjoint boundary conditions (2.3) for Sturm-Liouville equations (2.1).

Remark 1. *The canonical forms of self-adjoint boundary conditions for Sturm-Liouville equation (2.1) are critical for the theoretical investigation of the eigenvalues $\lambda_n(\gamma, K)$ or $\lambda_n(\alpha, \beta)$ of any self-adjoint operator S, as well as for their numerical computation as functions of these parameters. The properties of eigenvalue functions and the dependence of the eigenvalues and eigenfunctions on the boundary conditions are now well understood due to the voluminous literature of the second order Sturm-Liouville problems.*

For example, all the eigenvalues of any given self-adjoint operator S determined by the separated boundary conditions (2.8) are simple. And those of the coupled conditions (2.7) when $\gamma \neq 0$, are also simple and are continuous functions of the parameters $\alpha,\ \beta,\ \gamma$.

On the other hand the eigenvalues of S determined by the coupled conditions (2.7) when $\gamma = 0$ may be simple or double and they are not continuous functions of K. It is an open problem to *determine how many eigenvalues are simple and how many are double for a given boundary condition when $\gamma = 0$.*

3. SYMMETRIC DIFFERENTIAL EXPRESSIONS M

In 2019 Bao-Sun-Hao-Zettl introduced a class of skew-diagonal complex matrices $C = C_n = [c_{r,s}]_{r,s=1}^n \in M_n(\mathbb{C})$, $n = 2k,\ k > 1$ satisfying

$$C^* = -C = C^{-1},$$
$$C_n = \begin{pmatrix} 0 & C_{12} \\ -C_{12}^* & 0 \end{pmatrix}$$

Note that

$$E = E_n = ((-1)^r \delta_{r,n+1-s})_{r,s=1}^n$$

is a special case of C.

General quasi-differential epressions generated by E were introduced by Shin in 1938 but only a very special case of these were used by Naimark in his well known book. He mentioned the existence of the Shin expressions in a footnote of his book but did not use them. Other special cases of E, more general then the one used by Naimark, were used to generate quasi-differential expressions by many authors including

Barrett, Glazman, Kogan, Beketov, Reid, Stone, Walker, Weil, Hinton

In 1965 the Shin expressions were rediscovered by Zettl in slightly different but equivalent form.

Definition 1. *Let $Q = [q_{r,s}]_{r,s=1}^n \in M_n(L^1_{loc}(J)),\ J = (a,b), -\infty \le a < b \le \infty$. For $n = 2k,\ k \ge 1$ define*

$$\begin{aligned} Z_n(J) := \{Q = [q_{r,s}]_{r,s=1}^n \in M_n(L^1_{loc}(J)),\ & q_{r,r+1} \neq 0 \ \text{a.e. on } J; \\ & q_{r,r+1}^{-1} \in L^1_{loc}(J),\ 1 \le r \le n-1; \\ & q_{r,s} = 0 \quad \text{a.e. on } J,\ 2 \le r+1 < s \le n; \\ & q_{r,s} \in L^1_{loc}(J),\ s \neq r+1,\ 1 \le r \le n-1\}. \end{aligned}$$

If

$$Q = Q^+ := -C^{-1} Q^* C,$$

i.e.,

$$q_{r,s} = c_{r,n+1-r}\ \overline{q}_{n+1-s,n+1-r}\ c_{n+1-s,s},$$

where $C = [c_{r,s}]_{r,s=1}^n \in M_n(\mathbb{C})$. Then the matrix Q is called C-symmetric. For $Q \in Z_n(J)$, we define the r-th $(0 \le r \le n)$ quasi-derivative of y:

$$y^{[0]} = y\ (y \in V_0),\ V_0 := \{y : J \to \mathbb{C},\ y \text{ is measurable}\}$$

and

$$V_r = \{y \in V_{r-1} : y^{[r-1]} \in AC_{loc}(J),\ r = 1, 2, \ldots, n\},$$
$$y^{[r]} = q_{r,r+1}^{-1}[(y^{[r-1]})' - \sum_{s=1}^{r} q_{r,s} y^{[s-1]}] \qquad (y \in V_r),$$

where $q_{n,n+1} := c_{n,1}$.

If Q is C-symmetric then the expression $M = M_Q$ is called a C-symmetric quasi-differential expression. Since $M_Q^{++} = M_Q$ with $M_Q^{+} := M_{Q^+}$, M_Q is a symmetric differential expression.

4. **SELF-ADJOINT BOUNDARY CONDITIONS**

For n=2k, k>1**,** there are exactly three types of self-adjoint boundary conditions :

separated, coupled, and mixed

Theorem 1. *Consider the differential equation*

$$My = \lambda wy,\ \lambda \in \mathbb{C},\ J = (a,b),\ -\infty \le a < b \le +\infty,$$

with boundary conditions

$$AY(a) + BY(b) = 0,\ Y = \left[\begin{array}{cccc} y^{[0]} & y^{[1]} & \cdots & y^{[n-1]} \end{array}\right]^T,$$

where M is a C-Symmetric differential expression of order $n = 2k$, $k > 1$, and the matrices A, $B \in M_n(\mathbb{C})$ satisfy

$$ACA^* = BCB^*,$$

where C satisfies $C^* = -C = C^{-1}$. Then

(1)
$$k \le rank(A) \le n,\ \ k \le rank(B) \le n.$$

(2) for any r, $0 \le r \le$ k, if $rank(A) = k + r$, then $rank(B) = k + r$.
$$\text{if } rank(A) = k + r, \text{ then } rank(B) = k + r.$$

(3) Thus the boundary conditions are separated when $r = 0$, mixed when $1 \le r < k$, and coupled when $r = k$.

The next theorem states the characterization of the self-adjoint boundary conditions for regular problems. This theorem has been extended to the singular case; see the Comments Section below.

Theorem 2. *Consider the differential equation*

$$My = \lambda wy \text{ on } (a,b)$$

where M is a C-symmetric quasi-differential expression of order $n = 2k$, $k > 1$, and the boundary condition

$$AY(a) + BY(b) = 0,\ Y = \left[\begin{array}{cccc} y^{[0]} & y^{[1]} & \cdots & y^{[n-1]} \end{array}\right]^T,$$

where $A,\ B \in M_n(\mathbb{C})$ satisfy

$$rank(A) = rank(B) = n,\ AC_nA^* = BC_nB^*.$$

Then this coupled boundary condition is self-adjoint if and only if

$$Y(b) = e^{\mathrm{i}\xi}KY(a),\ K = -C\hat{A}C,\ -\pi < \xi \le \pi,$$

where $|\det(K)| = 1,\ \hat{A} = [\bar{b}_{r,s}]_{r,s=1}^n$.

Remark 2. *The characterization of this theorem requires the computation of the inverse of the boundary condition matrix A. In the notation $\hat{A} = [\bar{b}_{r,s}]_{r,s=1}^n$ recall the well known Laplace construction of the inverse of a non singular matrix:*

[*Matrix Inverse*] For $A = [a_{r,s}]_{r,s=1}^n \in M_n(\mathbb{C})$, let $A_{r,s}$ denote the submatrix of A obtained by removing row r and column s from A. Let

$$b_{r,s} = (-1)^{r+s} \det(A_{r,s}),$$

(1) and recall that if $\det(A) \neq 0$, then

$$A^{-1} = \frac{1}{\det(A)}([b_{s,r}]_{r,s=1}^n).$$

Remark 3. *This construction is consistent with the second order case and works for all orders $n = 2k,\ k \geq 1$. In other words this theorem extends the second order case $k = 2$ to the higher order cases $n = 2k,\ k > 1$.*

5. A Symplectic Group and Canonical Forms

Recall the class of skew-diagonal matrices $C = [c_{r,s}]_{r,s=1}^n \in M_n(\mathbb{C})$, $n = 2k,\ k \geq 1$ satisfying

$$C^* = -C = C^{-1},$$

i.e., C can be written as the form

$$C = \begin{bmatrix} 0 & C_k \\ -C_k^* & 0 \end{bmatrix},$$

with $C_k = [c_{r,k+s}]_{r,s=1}^k \in M_k(\mathbb{C})$ satisfying

$$c_{r,k+s}\bar{c}_{r,k+s} = 1, \text{ for } r = k+1-s,$$
$$c_{r,k+s} = 0, \text{ otherwise.}$$

Definition 2. *Let $C = C_n$ $(n = 2k,\ k \geq 1)$ be a complex skew-diagonal matrix as defined above. Define*

$$G_n(C) = \{A \in GL_n(\mathbb{C}) :\ ACA^* = C\},$$

where $GL_n(\mathbb{C})$ denotes the group of all nonsingular $n \times n$ matrices of complex numbers.

Theorem 3. $G_n(C)$ *is a group with the following properties:*

(1) $I = I_n \in G_n(C)$, is the identity of the group $G_n(C)$.
(2) If $A \in G_n(C)$ then A^* is in $G_n(C)$.
(3) If $A,\ B \in G_n(C)$, then $AB \in G_n(C)$
(4) If $A \in G_n(C)$, then $A^{-1} \in G_n(C)$.
(5) If $A \in G_n(C)$, then $|\det(A)| = 1$.
(6) If $A \in G_n(C)$, then $\det(A) = e^{i\xi},\ -\pi < \xi \leq \pi$.

Remark 4. *Note that*

$$J_n = \begin{bmatrix} 0 & I_k \\ -I_k & 0 \end{bmatrix}$$

has the property that

$$J_n^{-1} = -J_n = J_n^*,$$

and generates the ***standard*** *symplectic group J_n which is a special case of the C-symplectic group $G_n(C)$ used here.*

6. GENERAL COMMENTS

(1) The problem of finding canonical forms for the self-adjoint boundary conditions of operators of order $n = 2k$, $k > 1$, was an open problem for more than 100 years.

(2) It is interesting to note that the same matrix C which constructs the symmetric differential expressions M also characterizes the self-adjoint operators S.

(3) The characterization of self-adjoint boundary conditions given here for regular problems extends readily to singular problems. Only the conditions at the regular endpoints have to be changed to singular 'Lagrange bracket' conditions.

7. **Deficiency Indices**

For differential equations of order $n = 2k$, $k > 1$, with real coefficients, in an attempt to generalize the second order case, in several papers in the years 1938-1942 for equations of order $2k$, $k > 1$, Shin came to the conclusion that there are only two deficiency indices $d = k$ *and* $d = 2k$.

In a seminal paper in 1950 Glazman proved that all values between k and $2k$ are realized.

In 1966, for differential equations with complex coefficients of order $n = 2k$, $k > 1$, McLeod showed there are two deficiency indices d^+ and d^- which, in general, are different.

What are their possible values?

This question received a great deal of attention from 1966 to 2018 when it was solved by Aiping Wang and Anton Zettl.

In 1975 and 1976 Kogan and Rofe-Beketov proved that all values of d^+ and d^- which satisfiy the well known inequalities and differ by no more than 1 are realized.

In 1978 and 1979 Gilbert proved that the difference between d^+ and d^- can be arbitrarily large provided that the order of the differential equation is large enough. This result gave considerable support to the conjecture that all values of d^+ and d^- are realized as long as they satisfy the known inequalities.

It was known as the Deficiency Index Conjecture.

In Section V of their 1999 AMS book “Boundary Value Problems and Symplectic Algebra for Ordinary Differential and Quasi-Differntial Operators” Everitt and Markus state; ... “the mathematical signifigance of **The Deficiency Index Cojecture** ... is essential for the satisfactory completion of the conclusions of Section V.” (Section V means Chapter 5.) Thus the proof of the **Deficiency Index Conjecture** in the AMS book **“Ordinary Differential Operatorss”** by Wang-Zettl gives a satisfactory completion of the conclusions of Section V of the Everitt-Markus book.

References

- Bao, Sun, Hao, Zettl, “Canonical Forms of Boundary Conditions of Regular and Singular Differential Operators,” Electronic Journal of Differential Equations, 2022 (to appear).
- Anton Zettl, “Recent Developments in Sturm-Liouville Theory”, Studies in Mathematics, Vol. 76, De Gruyter, 2021.
- Aiping Wang and Anton Zettl, “Ordinary Differential Operators,” Mathematical Surveys and Monographs, Vol. 245, American Mathematical Society, 2019.