

ABSTRACT

Boundary Conditions associated with Left-Definite Theory and the Spectral
Analysis of Iterated Rank-One Perturbations

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This dissertation details the development of several analytic tools that are used to apply the techniques and concepts of perturbation theory to other areas of analysis. The main application is an efficient characterization of the boundary conditions associated with the general left-definite theory for differential operators. This theory originated with the groundbreaking work of Littlejohn and Wellman in 2002 which fully determined the ‘*left-definite domains*’ and spectral properties of powers of self-adjoint Sturm–Liouville operators associated with classical orthogonal polynomials. We will study how the left-definite domains associated with these operators can be explicitly described by classical boundary conditions.

Additional applications are made to infinite rank perturbations by successively introducing rank-one perturbations to a self-adjoint operator with absolutely continuous spectrum. The absolutely continuous part of the spectral measure of the constructed operator is controlled and estimated.

Boundary Conditions associated with Left-Definite Theory and the Spectral
Analysis of Iterated Rank-One Perturbations

by

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To my parents,
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CHAPTER ONE

Introduction

Perturbation theory addresses a question that underlies deep concerns in several fields of mathematics:

Given a mathematical construct, what happens to its key ingredients when it is changed by a certain amount?

For instance, chaos theory in topology and invariant theory in representation theory are each formulated around answering this question in various ways. In analysis, one way to ask the question is: How does a perturbation change the spectrum of an operator? The declaration of the spectrum as our key ingredient narrows our question to certain classes of operators: self-adjoint, unitary and normal. This restriction of our attention is also natural because these operators more closely model physical scenarios. Namely, self-adjoint operators correspond to closed physical systems, i.e. where energy remains constant and none is gained or lost from the environment. The investigation of this question can take many different forms, only a few of which are described or hinted at in this dissertation. Indeed, even the concept of a perturbation must be clarified before any exploration can take place.

The origins of modern perturbation theory are expressed in Tosio Kato's 1966 book *Perturbation Theory for Linear Operators* [37], and rank-one perturbations are in many ways the simplest type of perturbation described therein. Namely, given a self-adjoint operator T on a separable Hilbert space \mathcal{H} consider the *family of self-adjoint rank-one perturbations* by a vector $\varphi \in \mathcal{H}$:

$$T_\alpha = T + \alpha \langle \cdot, \varphi \rangle \varphi, \quad \alpha \in \mathbb{R}.$$

If the vector f is in the domain of T , the operator T_α simply applies T to f and adds a scalar multiple of the vector projection of f onto φ . This means that only

vectors whose inner product with φ are nonzero are of interest, so only the cyclic subspace spanned by φ under T is analyzed. The presence of only a single vector φ , and single parameter α , identify this as a rank-one perturbation. For details beyond this informal discussion, see Section 2.1 below.

A rank-one perturbation, as described above, is not only a compact operator, it is also Hilbert–Schmidt, trace class and even of finite rank (rank-one). These classifications suggest that our study of these objects should be manageable, yet their deeply subtle perturbation-theoretic properties also possess far-reaching implications. Barry Simon sums up the their appeal in his book *Trace Ideals and Their Applications*, [61]:

“The cynic might feel that I have finally sunk to my proper level. I started with quantum field theory, analysis in infinitely many variables. That was too hard so I switched to the N -body Schrödinger equation; but that was too hard so I switched to the one-body, then one-dimensional, then discrete one-dimensional. Finally to rank-one perturbations – maybe something so easy that I can say something useful! Alas, we’ll see even this is hard and exceedingly rich.”

Simon’s quote illustrates the reduction of many more difficult problems to the essential investigation of rank-one perturbations, although the theory does indeed remain very difficult. For example, a description of the so-called singular continuous spectrum of the perturbed operator T_α in terms of properties of the unperturbed operator T is unknown [61]. Moreover, beyond the realms of mathematical physics and spectral analysis of self-adjoint operators, the study of rank-one perturbations is connected to many interesting topics in analysis, see e.g. [14, 44, 47, 58] and the references within.

The difficulties are compounded further when introducing more vectors and parameters into the the family of perturbations, as hinted at by Simon. In particular, an exceedingly rich research area of mathematical physics is the spectral analysis of Anderson-type Hamiltonians, which include infinite-rank perturbations. This fascination comes from a conjecture made by P.W. Anderson in 1958 that has spawned incredible interest in the field by mathematical physicists:

Conjecture (Extended States, Anderson [5]). Sufficiently large impurities in a semiconductor leads to spatial localization of electrons.

Perturbations in Anderson-type Hamiltonians are non-compact operators with probability one, so the hypotheses in classical perturbation theory are not general enough to cover this problem. The connection between rank-one perturbations and infinite-rank perturbations is therefore somewhat unexpected, but they have been shown to have close ties nonetheless [45, 62, 63]. Chapter 4, while not directly addressing the Extended States Conjecture, builds upon these connections by iteratively introducing rank-one perturbations to an operator in order to form an object similar to an Anderson-type Hamiltonian.

Somewhere between the extremes of rank-one perturbations and Anderson-type Hamiltonians lie finite rank perturbations. Chapter 3 focuses on their applications to left-definite theory. This theory was introduced in the groundbreaking paper of Littlejohn and Wellman in 2002 [49] and describes a scale of nested Hilbert spaces associated with some differential operators. These nested Hilbert spaces are the domains of the powers of the original differential operator and can be analyzed using various techniques from self-adjoint extension theory and Sturm–Liouville theory. While perturbation theory is not explicitly used in our analysis, the benefit of a perturbation-theoretic mindset in this field is significant. Further applications are still emerging, but the fundamental nature of our initial question implies that our work is just beginning.

1.1 Notation

We use ℓ to denote differential expressions (on a separable Hilbert space \mathcal{H}), usually general Sturm–Liouville expressions in symmetric form. Specific differential expressions may use subscripts to distinguish them. Sets and spaces are generally

denoted with “mathcal”; the Hilbert space \mathcal{H} , the minimal domain \mathcal{D}_{\min} , the defect spaces \mathcal{D}_+ and \mathcal{D}_- , etc.

The notation $\{\ell, \mathcal{X}\}$ is used to refer to an operator acting via ℓ on the domain \mathcal{X} . Since we work with unbounded operators, they are defined only on dense subspaces $\mathcal{X} \subsetneq \mathcal{H}$. The maximal domain is denoted by \mathcal{D}_{\max} , with $\mathcal{D}_{\max}(\ell)$ occasionally used to emphasize the expression. Boldface letters are used for operators and matrices that are related to differential expressions, as different domains and expressions become easily confused. Namely, Sections 2.2, 2.3, 2.4, and all of Chapter 3 use this convention. However, in other Chapters where the domains are clearly stated, this notation is avoided for simplicity.

We abbreviate the maximal and minimal operators by \mathbf{L}_{\max} and \mathbf{L}_{\min} , i.e. $\mathbf{L}_{\max} = \{\ell, \mathcal{D}_{\max}\}$ and $\mathbf{L}_{\min} = \{\ell, \mathcal{D}_{\min}\}$. Similarly, $\mathbf{L} = \{\ell, \mathcal{D}_{\mathbf{L}}\}$ is used to denote self-adjoint operators in this context. It is also common for powers \mathbf{L}^n of operators to be examined, e.g. we consider the left-definite operator induced by the expression ℓ^n . Abusing notation, we write $\mathbf{L}_{\max}^n = \{\ell^n, \mathcal{D}_{\max}^n\}$ where $\mathcal{D}_{\max}^n := \mathcal{D}_{\max}(\ell^n)$, to express these powers. Further, let $[\cdot, \cdot]$ denote a general sesquilinear form, and $[\cdot, \cdot]_n$ stand for the sesquilinear form associated with ℓ^n . Generally, we let (m, m) be the deficiency indices of \mathbf{L}_{\min} . It is then noted that the deficiency indices of \mathbf{L}_{\min}^n amount to (nm, nm) .

The domain of a general operator A , not necessarily related to a differential expression, is referred to by $\mathcal{D}(A)$. Unitary equivalence (i.e. $UAU^{-1} = B$ for some unitary operator U) of the operators A and B will be denoted by $A \sim B$. Similarly, the notation

$$A \sim B(\text{mod } \textit{Class } X)$$

is used if there exists a unitary operator U such that $UAU^{-1} - B$ is an element of *Class X*. The *Class X* can be any class of operators, e.g. compact, trace class, or finite rank operators.

CHAPTER TWO

Background

The analytic tools developed for applications in future chapters require knowledge of both perturbation theory and the subjects of these applications. Section 2.1 reviews selected results from perturbation theory. For the sake of brevity, only some of the operator theoretic and functional analytic foundations of these results are discussed. Additional details can be found in [1, 4, 14, 37, 44, 47]. The most widely used results stem from Aronszajn–Donoghue theory. In particular, explicit formulas for both the pure point and absolutely continuous part of perturbed spectra are stated. An in depth discussion of Aronszajn–Donoghue theory can be found in [61]. Unitary perturbations are omitted in this discussion because they are not used in later chapters. Readers interested in these descriptions should consult [14, 58] for excellent surveys. This background is supplemented in Subsection 2.1.1 by a summary of how Hilbert scales are used to allow for perturbation vectors outside of the original Hilbert space.

Sturm–Liouville differential operators are classical models used throughout many areas of pure and applied mathematics, not least because some of them have naturally occurring eigenfunctions which form systems of orthogonal polynomials. Section 2.2 describes the setup of these differential operators and some basic facts about them. This theory is particularly pertinent to the general framework described in Section 3.4. The classification of endpoints in Subsection 2.2.1 explains how deficiency indices are related to behavior of coefficient functions at endpoints. The discussion provides more context in order to better understand how deficiency indices are used in Chapter 3.

Left-definite theory provides a scheme for taking a (Sturm–Liouville) differential operator and generating a scale of Hilbert spaces which involve the domains of compositions of the operator. Section 2.3 mainly follows the classical results contained in [49], and includes the structure of left-definite spaces as well as key facts about their spectra. An underlying concern of this study is the assurance that all operators are self-adjoint, so their spectra can be studied. The self-adjoint extension theory in Section 2.4 follows the classical text of Naimark [54] and details the abstract construction of such operators when given a formally symmetric differential expression. It culminates in Glazman–Krein–Naimark theory (Subsection 2.4.1), which expresses these constructions as varying boundary conditions given by functions in the domain of the expression.

Finally, the iterated operator constructed in Chapter 4 is deemed similar to an Anderson-type Hamiltonian, yet possesses a few notable differences. In order to discern these differences and present the goal of the construction, Section 2.5 briefly introduces Anderson-type Hamiltonians.

2.1 Perturbation Theory

Perturbation theory is generally formulated around answering a refinement of the question posed in the Introduction:

Given some information about the spectrum of an operator A , what can be said about the spectrum of the operator $A + B$ when B is in some operator class?

Equivalently, we can ask if properties of parts of the spectrum can be preserved under certain changes. The answer, of course, varies wildly depending on the class of operators the perturbation B is taken from.

A review of the most well-known answers to this question necessitates a description of spectral measures and their various decompositions. Let μ be a positive

measure on $[a, \infty)$ for some $a > -\infty$ with

$$\int \frac{d\mu(\lambda)}{|\lambda| + 1} < \infty. \quad (2.1.1)$$

This assumption is somewhat restrictive, but is necessary for the study of Borel transforms. It is also satisfied by spectral measures that arise from rank-one perturbations when the perturbation vector $\varphi \in \mathcal{H}_{-1}$, as described in Subsection 2.1.1. The condition that the support of μ is bounded below can be relaxed somewhat, but does hold in the applications in Chapters 3 and 4, and simplifies further details slightly.

Adherence to (2.1.1) allows us to define the *Borel transform* of μ as

$$F(z) := \int_{\mathbb{R}} \frac{d\mu(\lambda)}{\lambda - z} \quad (z \in \mathbb{C} \setminus (\text{supp } \mu)).$$

Interestingly, another function,

$$G(x) := \int_{\mathbb{R}} \frac{d\mu(y)}{(y - x)^2} \quad (x \in \mathbb{R} \setminus (\text{supp } \mu)),$$

also plays a central role. This auxiliary transform captures some properties of the derivative (with respect to z) of the Borel transform as z approaches the real axis. Indeed, boundary values of $F(z)$, as $z = x + i\epsilon$ approaches points x in the support of μ , are the primary instrument to discern spectral properties of μ . See [61] for a more detailed discussion.

It is often more convenient to consider slight variations of the Borel transform. For instance, the Cauchy transform of a measure μ that adheres to (2.1.1) is defined as

$$K\mu(z) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{d\mu(t)}{t - z}, \quad z \in \mathbb{C}_+,$$

and is obtained from the Borel transform by restricting the domain to the upper half of the complex plane and multiplying by $1/\pi$. The connection between the Cauchy transform and the spectral theory of rank-one perturbations is particularly well developed, see e.g. [14, 44, 47, 58] and this connection is exploited in several of the

previous results. It is also heavily relied upon when unitary rank-one perturbations are considered. In order to avoid difficulties with convergence, it is standard to introduce an alternative definition of the Cauchy transform

$$K_1\mu(z) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{1}{t-z} - \frac{t}{t^2+1} d\mu(t), \quad z \in \mathbb{C}_+.$$

While these two transforms locally behave alike, the advantage of introducing this alternative definition is that it is possible to define $K_1\mu$ for more general measures μ (because the kernel decays faster at infinity). It is worth mentioning that (for μ such that $K\mu$ is defined on \mathbb{C}_+) the real part of $K_1\mu$ differs from the conjugate Poisson integral by a finite additive constant. The use of the K_1 transform in the literature of rank-one perturbations both implies and stems from connections to Ordinary Differential Equations. Specifically, it is a real analog of the Nevanlinna–Herglotz representation of the Weyl m -function in Sturm–Liouville theory.

The measure μ used in our applications will always be a spectral measure. To this end, let T be a self-adjoint operator (bounded or unbounded) on a separable Hilbert space \mathcal{H} . The operator T will be called cyclic when it possesses a vector φ such that

$$\mathcal{H} = \overline{\text{span}\{(T - \lambda\mathbf{I})^{-1}\varphi : \lambda \in \mathbb{C} \setminus \mathbb{R}\}}, \quad (2.1.2)$$

where the closure is taken with respect to the Hilbert space norm. In this case, the vector φ is also called cyclic. The formal expression

$$T_\alpha = T + \alpha \langle \cdot, \varphi \rangle_{\mathcal{H}} \varphi \quad \text{for} \quad \alpha \in \mathbb{R} \quad (2.1.3)$$

represents the *rank-one perturbation of a self-adjoint operator T with cyclic vector φ* . A simple consequence of these definitions is that φ is also a cyclic vector of the operator T_α for all $\alpha \in \mathbb{R}$, see [46] for more about cyclicity. The supposition that T is cyclic is not a restriction, as otherwise we simply decompose $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ such that φ is cyclic for T on \mathcal{H}_1 and T is left unchanged by the perturbation when restricted

to \mathcal{H}_2 . The spectral measure of T_α with respect to the cyclic vector φ will be denoted by μ_α . Explicitly, the spectral theorem defines μ_α via

$$\langle (T_\alpha - z\mathbf{I})^{-1}\varphi, \varphi \rangle_{\mathcal{H}} = \int_{\mathbb{R}} \frac{d\mu_\alpha(t)}{t - z} \quad \text{for all } z \in \mathbb{C} \setminus \mathbb{R}.$$

In other words, T is unitarily equivalent to multiplication by the independent variable on an $L^2(\mu_\alpha)$ space with non-negative Radon measure μ_α , the *spectral measure*, supported on \mathbb{R} . The spectral measure of the unperturbed operator T , μ_0 , is often used as a comparison to the spectral measure μ_α . Therefore, we use the convention that $\mu_0 = \mu$ for simplicity. This means that T can be written as M_t , multiplication by the independent variable on $L^2(\mu)$. The vector φ is then represented by the function that is identically equal to the constant function one on $L^2(\mu)$.

There are numerous decompositions of the spectrum used throughout the literature, so we clarify our definitions here. The Lebesgue/Radon–Nikodym decomposition can be applied to each spectral measure, yielding $d\mu = w(x)dx + d\mu_s$. Here, $w \in L^1_{\text{loc}}(\mathbb{R})$ is the Radon–Nikodym derivative of μ with respect to Lebesgue measure. The unitary equivalence between T and M_t involves a unitary intertwining operator. Explicitly, this is the unitary operator U such that $UTU^{-1} = M_t$. We refer to the operator U as the unitary intertwining operator in this scenario. This unitary equivalence gives rise to the corresponding orthogonal components of the operator $T = T_{\text{ac}} \oplus T_s$. The singular part can be further decomposed into singular continuous μ_{sc} and pure point μ_{pp} parts. Here, μ_{pp} consists of point masses at the eigenvalues of T and $\mu_{\text{sc}} = \mu_s - \mu_{\text{pp}}$. The spectrum is denoted by $\sigma(T)$ and is the (closed) $\text{supp}(\mu)$. The set of all real numbers x that are isolated eigenvalues of finite multiplicity for T is defined to be the discrete spectrum, denoted $\sigma_d(T)$. The essential spectrum of T is the complement of the discrete spectrum, denoted $\sigma_{\text{ess}}(T) = \sigma(T) - \sigma_d(T)$.

The spectral theorem now translates the rank-one perturbation problem to

$$\tilde{T}_\alpha = M_t + \alpha \langle \cdot, \mathbf{1} \rangle_{L^2(\mu)} \mathbf{1}. \quad (2.1.4)$$

Therefore, we identify $\mathcal{H} = L^2(\mu)$ and use $\tilde{T}_\alpha = T_\alpha$ for brevity of notation. The presence of a different unitary intertwining operator relating the operators T_α and M_s , on their respective spaces $\mathcal{H} = L^2(\mu)$ and $L^2(\mu_\alpha)$, begs the question whether we can say anything about an operator relating the spaces $L^2(\mu)$ and $L^2(\mu_\alpha)$. This question was answered in a paper of Liaw and Treil [47, Theorem 2.1]. The Theorem extends to all of $L^2(\mu)$, but a simpler version is presented here.

Theorem 2.1.1 (Representation Theorem). *The spectral representation $V_\alpha : L^2(\mu) \rightarrow L^2(\mu_\alpha)$ of T_α is given by*

$$V_\alpha f(s) = f(s) - \alpha \int \frac{f(s) - f(t)}{s - t} d\mu(t)$$

for all compactly supported C^1 functions f .

The following theorem provides more evidence for the historical connection enjoyed by perturbation theory and Sturm–Liouville theory. It was proven first by Aronszajn for boundary condition dependence of the spectrum for Sturm–Liouville operators and later extended to rank-one perturbations by Donoghue [7, 18]. The theorem characterizes the perturbed operator’s pure point and absolutely continuous spectra. The result is the most dynamic tool available in perturbation theory and will be heavily used in later sections.

Theorem 2.1.2 (Aronszajn–Donoghue, see e.g. [61]). *For $\alpha \neq 0$ ($\alpha = \infty$ allowed with $\infty^{-1} = 0$), define*

$$S_\alpha = \{x \in \mathbb{R} \mid F(x + i0) = -\alpha^{-1}; G(x) = \infty\},$$

$$P_\alpha = \{x \in \mathbb{R} \mid F(x + i0) = -\alpha^{-1}; G(x) < \infty\},$$

$$L = \{x \in \mathbb{R} \mid \operatorname{Im} F(x + i0) \neq 0\}.$$

Then we have

$$(1) \{S_\alpha\}_{\alpha \neq 0; |\alpha| \leq \infty}, \{P_\alpha\}_{\alpha \neq 0; |\alpha| \leq \infty} \text{ and } L \text{ are mutually disjoint.}$$

(2) P_α is the set of eigenvalues of A_α . In fact,

$$(d\mu_\alpha)_{\text{pp}}(x) = \sum_{x_n \in P_\alpha} \frac{1}{\alpha^2 G(x_n)} \delta(x - x_n), \alpha < \infty,$$

$$(d\rho_\infty)_{\text{pp}}(x) = \sum_{x_n \in P_\infty} \frac{1}{G(x_n)} \delta(x - x_n), \alpha = \infty.$$

(3) $(d\mu_\alpha)_{\text{ac}}$ is supported on L , $(d\mu_\alpha)_{\text{sc}}$ is supported on S_α .

(4) For $\alpha \neq \beta$, $(d\mu_\alpha)_s$ and $(d\mu_\beta)_s$ are mutually singular.

The case $\alpha = \infty$ is known as infinite coupling, and needs to be treated differently, but these details are avoided here. The main reference for this scenario is work by Gesztesy and Simon which is explained in our context in [28, 61]. The last part of the result says that the singular part of rank-one perturbations must move when the perturbation parameter α is changed. We also point out that a description of the singular continuous spectrum is still outstanding. In fact, the ‘minimal’ support of $(\mu_\alpha)_{\text{sc}}$ is not known, see e.g. [14, 47, 61], let alone a characterization of $(\mu_\alpha)_{\text{sc}}$. The lack of this characterization is widely regarded as the largest missing piece of the theory for rank-one perturbations.

The absolutely continuous part of the perturbed operator, $(\mu_\alpha)_{\text{ac}}$, can be explicitly computed using the following Lemma.

Lemma 2.1.3 (see e.g. [61]). *Let $F(z)$ be the Borel transform of a measure μ obeying (2.1.1). Let $\beta \in \mathbb{R}$, $x \in \mathbb{R}$, and $x + i0 = \lim_{\beta \downarrow 0} (x + i\beta)$. Standard harmonic analysis says these limits exist and are finite for a.e. x . Then we have*

$$(1) \quad \text{Im } F(x + i\beta) = \int_{\mathbb{R}} \frac{\beta}{(x - y)^2 + \beta^2} d\mu(y),$$

$$(2) \quad \text{Im } F_\alpha(z) = \frac{\text{Im } F(z)}{|1 + \alpha F(z)|^2}, \text{ and}$$

$$(3) \quad d(\mu_\alpha)_{\text{ac}}(x) = \pi^{-1} \text{Im } F_\alpha(x + i0) dx.$$

The support of the a.c. part of the perturbed spectral measure is curiously revealed to be independent of the parameter α in Aronszajn–Donoghue theory. This is really a consequence of the famous Kato–Rosenblum Theorem, which can be easily proven in the context of rank-one perturbations using the previous Lemma. However, it is presented here in the more general sense, as it provides a partial answer to our main question at the beginning of the section

Theorem 2.1.4 (Kato–Rosenblum, see e.g. [37]). *If for two self-adjoint operators we have $A \sim B(\text{mod trace class})$ then their absolutely continuous parts are unitarily equivalent, i.e. $A_{\text{ac}} \sim B_{\text{ac}}$.*

Recall the use of $A \sim B$ to denote the unitary equivalence of the operators A and B , as explained in the Notation Section 1.1. The Kato–Rosenblum Theorem is also the first positive result to our question posed at the beginning of the section. More can be said of the spectral connections when the perturbations come from other operator classes.

Theorem 2.1.5 (Weyl–von Neumann, see e.g. [37]). *The essential spectra of two self-adjoint operators A and B satisfy*

$$\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B) \text{ if and only if } A \sim B \text{ (mod compact operators).}$$

Remark. Carey and Pincus [13] found a complete characterization of when $A \sim B(\text{mod trace class})$ in terms of the operators’ spectrum for self-adjoint A and B .

It is worth emphasizing that all of these theorems can be applied to rank-one perturbations, as they are classified as both trace class and compact operators.

This connection actually forms part of the proof of Theorem 2.1.2 above. In the case of purely singular measures the following theorem resembles a characterization for $A \sim B(\text{mod rank-one})$.

Theorem 2.1.6 (Poltoratski [57]). *Let $X \subset \mathbb{R}$ be closed. By $I_1 = (x_1; y_1), I_2 = (x_2; y_2), \dots$ denote disjoint open intervals such that $X = \mathbb{R} \setminus \bigcup I_n$. Let A and B be two cyclic self-adjoint completely non-equivalent operators with purely singular spectrum. Suppose*

$$\sigma(A) = \sigma(B) = X$$

and assume that for the pure point spectra of A and B we have

$$\sigma_{\text{pp}}(A) \cap \{x_1, y_1, x_2, y_2, \dots\} = \sigma_{\text{pp}}(B) \cap \{x_1, y_1, x_2, y_2, \dots\} = \emptyset.$$

Then we have

$$A \sim B(\text{mod rank-one}).$$

This theorem allows us to introduce absolutely continuous spectrum while retaining precise control of the Radon–Nikodym derivatives of the singular measure.

Finally, no treatise on perturbation theory, however brief, is complete without at least mentioning the five critical formulas of rank-one perturbation theory. The formulas don't arise during the investigations in later Chapters, but are used in the proofs of some of the previous results. While they are presented here for reference, it is hoped that readers will recognize some of their implications if motivated to use the theory ([61] includes their derivations and uses).

Theorem 2.1.7. *Let $\varphi \in \mathcal{H}$. Then, using the notation of this Section, the following formulas hold.*

$$(1) \text{ The Aronszajn–Krein formula: } F_\alpha(z) = \frac{F(z)}{1 + \alpha F(z)}.$$

$$(2) (T_\alpha - z)^{-1}\varphi = (1 + \alpha F(z))^{-1}(T - z)^{-1}\varphi.$$

$$(3) (T_\alpha - z)^{-1} = (T - z)^{-1} - \frac{\alpha}{1 + \alpha F(z)} \langle \cdot, (T - \bar{z})^{-1}\varphi \rangle (T - z)^{-1}\varphi.$$

$$(4) \text{ The Trace formula: } \text{Tr}[(T - z)^{-1} - (T_\alpha - z)^{-1}] = \frac{\alpha}{1 + \alpha F(z)} \langle \varphi, (T - z)^{-2}\varphi \rangle.$$

(5) If $f \in L^1(\mathbb{R}, dx)$, then $f \in L^1(\mathbb{R}, d\mu_\alpha)$ for a.e. α , and the Spectral Averaging formula holds:

$$\int \left(\int f(x) \mu_\alpha(x) \right) d\alpha = dx.$$

Aronszajn–Donoghue theory can also be used for unbounded operators T and in the so-called singular form bounded perturbations case. This means that the vector φ is not contained in the Hilbert space \mathcal{H} , but is rather taken from a larger space commonly denoted by $\mathcal{H}_{-1}(T)$. Throughout this dissertation all perturbation vectors will be taken from \mathcal{H} and $\|\varphi\|_{\mathcal{H}} = 1$. However, some knowledge of how these spaces are related is desirable as context for our discussion of Sturm–Liouville theory.

2.1.1 Scales of Hilbert Spaces

When considering perturbations like equation (2.1.3), it is sometimes convenient to loosen our restrictions on the perturbation vector φ to expand our possible applications. We say that the perturbation is *bounded* when the vector φ is from the Hilbert space \mathcal{H} . The previous section dealt exclusively with bounded perturbations. If $\varphi \notin \mathcal{H}$, we say the perturbation is *singular*. These perturbations are significantly more complicated; it is imperative to ensure that the perturbation is well-defined in order to extend the tools from the previous Section appropriately. The description here roughly follows that of [4], and the attentive reader should notice many similarities between the scale of spaces here and the scale in left-definite theory presented later.

Let T be a positive operator. Note that if T is a possibly unbounded self-adjoint operator on a separable Hilbert space \mathcal{H} , the positive operator defined by $|T| = (T^*T)^{1/2}$ can be considered. Alternatively, if T is bounded from below, the shifted operator $T + kI$, $k \in \mathbb{R}$ sufficiently large, suffices. We can now introduce the following scale of spaces.

Definition 2.1.8 ([4, Section 1.2.2]). For $s \geq 0$, define the space $\mathcal{H}_s(T)$ to be $\mathcal{D}(T^{s/2})$ with norm equal to the graph norm of the operator

$$\|\varphi\|_s = \|(T + 1)^{s/2}\varphi\|_{\mathcal{H}}.$$

The space $\mathcal{H}_s(T)$ equipped with the norm $\|\cdot\|_s$ is complete, and the adjoint spaces formed by the linear bounded functionals are defined as $\mathcal{H}_{-s}(T) = \mathcal{H}_s^*(T)$. The corresponding norm in the space $\mathcal{H}_{-s}(T)$ is thus defined by the formula

$$\|\varphi\|_{-s} = \left\| \frac{1}{(T + 1)^{s/2}} \varphi \right\|_{\mathcal{H}},$$

where the operator $1/(T + 1)^{s/2}$ is defined in the generalized sense. The *scale of Hilbert spaces associated with the self-adjoint operator T* is the collection of these $\mathcal{H}_s(T)$ spaces when $s \in \mathbb{Z}$.

Furthermore, it is easy to see that the spaces have the following nesting properties

$$\cdots \subset \mathcal{H}_2(T) \subset \mathcal{H}_1(T) \subset \mathcal{H} = \mathcal{H}_0(T) \subset \mathcal{H}_{-1}(T) \subset \mathcal{H}_{-2}(T) \subset \cdots$$

and that for every two s, t , $s < t$, the space $\mathcal{H}_t(T)$ is dense in $\mathcal{H}_s(T)$ in the norm $\|\cdot\|_s$. Indeed, the operator $(T + 1)^{t/2}$ defines an isometry from $\mathcal{H}_s(T)$ to $\mathcal{H}_{s-t}(T)$. Through the rest of the subsection, we will use the brackets $\langle \cdot, \cdot \rangle$ to denote both the scalar product in the Hilbert space \mathcal{H} and the action of the functionals. For instance, if $\varphi \in \mathcal{H}_{-s}(T)$, $\psi \in \mathcal{H}_s(T)$, then

$$\langle \varphi, \psi \rangle \equiv \left\langle \frac{1}{(T + 1)^{s/2}} \varphi, (T + 1)^{s/2} \psi \right\rangle,$$

where the brackets on the right hand side denote the scalar product. This is an example of a *Hilbert scale*, although there are other names throughout the literature when they are applied to other fields. For instance, the pairing of $\mathcal{H}_1(T)$, \mathcal{H} , and $\mathcal{H}_{-1}(T)$ is sometimes referred to as a *Gelfand triple* or *rigged Hilbert space*, and these

constructs may be more familiar to the reader. More details about Hilbert scales in general can be found in [42].

Rank-one perturbations of a given operator T arise most commonly when the vectors φ are bounded linear functionals on the domain of the operator T . Hence, we restrict our attention to $\mathcal{H}_{-2}(T)$, as $\mathcal{D}(T) = \mathcal{H}_2(T)$ and $\mathcal{D}(T)^* = \mathcal{H}_{-2}(T)$. The case where $\varphi \notin \mathcal{H}_{-2}$ has more complicated expressions which are the premises of [16, 43]. A more practical way to distinguish whether a perturbation vector φ is in $\mathcal{H}_{-1}(T)$ or $\mathcal{H}_{-2}(T)$ is still desired. If $\varphi \in \mathcal{H}_{-2}(T)$, the linear operator that appears in rank-one perturbations

$$\langle \cdot, \varphi \rangle \varphi : \mathcal{H}_2(T) \rightarrow \mathcal{H}_{-2}(T)$$

naturally defines the following positive sesquilinear form

$$\mathbf{V}_\varphi[\psi, \eta] = \langle \varphi, \psi \rangle \langle \eta, \varphi \rangle = \langle \varphi, \psi \rangle \overline{\langle \varphi, \eta \rangle} \quad (2.1.5)$$

for $\psi, \eta \in \mathcal{H}_2(T)$. This sesquilinear form allows for the further characterization of classes of singular perturbations.

Definition 2.1.9 ([4, Section 1.2.3]). The sesquilinear form $V[\psi, \eta]$ will be called *form bounded with respect to the operator T* if and only if the domain $\mathcal{D}(V)$ of the form is contained in the space $\mathcal{H}_1(T)$ and there exist two positive real constants C_1 and C_2 such that for any $\psi \in \mathcal{D}(V)$ the following estimate holds:

$$V[\psi, \psi] \leq C_1 \|\psi\|_1^2 + C_2 \|\psi\|_{\mathcal{H}}^2.$$

Recall that $\|\cdot\|_1$ and $\|\cdot\|_{\mathcal{H}}$ denote the norms in $\mathcal{H}_1(T)$ and $\mathcal{H}_0(T) = \mathcal{H}$ respectively. If the constant C_1 can be chosen arbitrarily small, the form V is said to be *infinitesimally form bounded with respect to the operator T* .

The next result characterizes form boundedness with respect to perturbation theory.

Lemma 2.1.10 ([4, Lemmas 1.2.1, 1.2.2]). *Let $\varphi \in \mathcal{H}_{-1}(T)$. The the sesquilinear form $\mathbf{V}_\varphi[\psi, \eta]$ is infinitesimally form bounded with respect to the operator T .*

However, if $\varphi \in \mathcal{H}_{-2}(T) \setminus \mathcal{H}_{-1}(T)$, then the sesquilinear form $\mathbf{V}_\varphi[\psi, \eta]$ is not form bounded with respect to the operator T .

It is worth pointing out that the five critical formulas in Theorem 2.1.7 have been altered to apply to $f \in \mathcal{H}_{-2}(T)$ and are presented in [4]. The infinite coupling that arises in Theorem 2.1.2 was also extended to $\varphi \in \mathcal{H}_{-1}(T)$ in [40]. Hence, the demarcation of singular perturbations into form bounded and not form bounded perturbations provides additional tools for exploration.

2.2 Sturm–Liouville Operators

Sturm–Liouville differential equations are common examples of ordinary differential equations that are used in many areas of pure and applied mathematics. Notably, they are the classical way to generate systems of solutions that are orthogonal polynomials with respect to some weight function and arise as important simplifications (Lax pairs) for some famous partial differential equations. Consider the classical Sturm–Liouville differential expression

$$-\frac{1}{w(x)} \left[\frac{d}{dx} p(x) \frac{d}{dx} + q(x) \right], \quad (2.2.1)$$

where the independent variable is x , $p(x), w(x) > 0$ a.e. on (a, b) and $q(x)$ real-valued a.e. on (a, b) for $-\infty \leq a < b \leq \infty$. Furthermore, $1/p(x), q(x), w(x) \in L^1_{\text{loc}}[(a, b), dx]$. Additional details about Sturm–Liouville theory can be found in [29, 66, 67]. These standard assumptions on the coefficient functions and endpoints will be assumed throughout this dissertation, and recall that the notation used here is described in Section 1.1.

The differential expression (2.2.1) can be viewed as a linear operator, mapping a function f to the function $\ell[f]$ via

$$\ell[f](x) := -\frac{1}{w(x)} \left(\frac{d}{dx} \left[p(x) \frac{df}{dx}(x) \right] + q(x)f(x) \right). \quad (2.2.2)$$

The unbounded operator acts on the Hilbert space $L^2[(a, b), w]$, endowed with the inner product $\langle f, g \rangle := \int_a^b f(x) \overline{g(x)} w(x) dx$. In this setting, the eigenvalue problem $\ell[f](x) = \lambda f(x)$ can be considered. The operators of interest, $\{\ell, L^2[(a, b), w]\}$, are also assumed to possess a set of orthogonal eigenfunctions that is complete in the domain for the purposes of Chapter 3. The expression $\ell[\cdot]$ defined in equation (2.2.2) has been well-studied, see [33] for an in-depth discussion of its relation to orthogonal polynomials. However, the operator $\{\ell, L^2[(a, b), w]\}$ is not self-adjoint a priori. Subsection 2.4.1 details the imposition of boundary conditions to ensure self-adjointness.

Furthermore, the operator $\ell^n[\cdot]$ is defined as the operator $\ell[\cdot]$ composed with itself n times, creating a differential operator of order $2n$. Every formally symmetric differential expression $\ell^n[\cdot]$ of order $2n$ with coefficients $a_k : (a, b) \rightarrow \mathbb{R}$ and $a_k \in C^k(a, b)$ for $k = 0, 1, \dots, n$ and $n \in \mathbb{N}$ has the *Lagrangian symmetric form*

$$\ell^n[f](x) = \sum_{j=1}^n (-1)^j (a_j(x) f^{(j)}(x))^{(j)}, \quad x \in (a, b). \quad (2.2.3)$$

Further details can be found in [19, Section XIII.2] or [52].

The classical differential expressions of Jacobi, Hermite, and Laguerre all admit such a representation, and are semi-bounded. *Semi-boundedness* is defined as the existence of a constant $k \in \mathbb{R}$ such that for all x in the domain of the operator \mathbf{A} the following inequality holds:

$$\langle \mathbf{A}x, x \rangle \geq k \langle x, x \rangle.$$

This additional property, combined with self-adjointness, allows for a continuum of nested Hilbert spaces to be defined within $L^2[(a, b), w]$ via the expressions $\ell^n[\cdot]$. Indeed, this continuum is a Hilbert scale, and many facts about the spectrum and the

operators can be deduced using this point of view (e.g. [17, 50]). More details about Hilbert scales can be found in [4, 42] and the previous discussion in Subsection 2.1.1. This particular Hilbert scale with self-adjoint operators that are semi-bounded is the topic of left-definite theory [49], part of which is explained in Section 2.3.

2.2.1 Classification of Endpoints

Sturm–Liouville operators are often classified by the amount of regularity present at their endpoints. The regularity of the endpoints determines how many boundary conditions are necessary to ensure self-adjointness of the operator.

Definition 2.2.1 ([29]). The differential expression ℓ is called *regular* at the endpoint a if $a \in \mathbb{R}$, and $1/p(x), q(x), w(x) \in L^1[(a, c), dx]$ for all $c \in (a, b)$. Otherwise, ℓ is said to be *singular* at a .

A first-order initial value problem can be solved at regular endpoints, making solutions of Sturm–Liouville differential expressions very well behaved. The spectrum of differential equations that are regular at both endpoints is discrete [4, 29, 54]. Singular endpoints give the possibility of absolutely continuous spectrum arising and are much more difficult to study. These singular endpoints can be sorted into two categories but a notational convention is necessary first.

Definition 2.2.2 ([29]). Let $f : (a, b) \rightarrow \mathbb{C}$ be a measurable function. It is said that f lies in $L^2[(a, b), w]$ *near* a , if there exists $c \in (a, b)$ such that $f \in L^2[(a, c), w]$. Similarly, f lies in $L^2[(a, b), w]$ *near* b , if there exists a $d \in (a, b)$ such that $f \in L^2[(d, b), w]$.

Theorem 2.2.3 (Weyl’s Alternative). *Exactly one of the following cases holds:*

- (1) *For every $z \in \mathbb{C}$, all solutions u of $(\ell - z)u = 0$ are in $L^2[(a, b), w]$ near b (resp. near a).*
- (2) *For every $z \in \mathbb{C}$, there exists at least one solution of $(\ell - z)u = 0$ which is not in $L^2[(a, b), w]$ near b (resp. near a). In this case, for each $z \in \mathbb{C}/\mathbb{R}$, there*

exists precisely one solution u_b (resp. u_a) of $(\ell - z)u = 0$ (up to constant multiples) which lies in $L^2[(a, b), w]$ near b (resp. near a).

Theorem 2.2.4. *In case (1) above, ℓ is said to be in the limit circle case (l.c.c.) at b (resp. at a). In case (2) above, ℓ is said to be in the limit point case (l.p.c.) at b (resp. at a).*

Additional details will be given at the end of Section 2.4, as endpoint classification directly determine the defect indices of symmetric Sturm–Liouville expressions. This discussion will be essential to Section 3.4, which details the most general results obtained during the investigation of boundary conditions associated with left-definite theory.

2.3 Left-Definite Theory

Left-definite theory deals primarily with the spectral theory of Sturm–Liouville differential operators. The terminology itself can be traced back to Weyl in 1910 [68]. A general framework for the left-definite theory of bounded-below, self-adjoint operators in a Hilbert space wasn't developed until 2002 in the landmark paper by Littlejohn and Wellman [49]. Specifically, the left-definite theory allows one to generate a scale of operators (by composition), and many spectral properties remain the same as the original. Recall that we will change our notation slightly in the next two Sections in order to avoid confusion over which domain each operator is acting on, in accordance with Section 1.1.

Let \mathcal{V} be a vector space over \mathbb{C} with inner product $\langle \cdot, \cdot \rangle$ and norm $\| \cdot \|$. The resulting inner product space is denoted $(\mathcal{V}, \langle \cdot, \cdot \rangle)$.

Definition 2.3.1 ([49, Theorem 3.1]). Suppose \mathbf{A} is a self-adjoint operator in the Hilbert space $\mathcal{H} = (\mathcal{V}, \langle \cdot, \cdot \rangle)$ that is bounded below by kI , where $k > 0$. Let $r > 0$. Define $\mathcal{H}_r = (\mathcal{V}_r, \langle \cdot, \cdot \rangle_r)$ with

$$\mathcal{V}_r = \mathcal{D}(\mathbf{A}^{r/2})$$

and

$$\langle x, y \rangle_r = \langle \mathbf{A}^{r/2}x, \mathbf{A}^{r/2}y \rangle \text{ for } (x, y \in \mathcal{V}_r).$$

Then \mathcal{H}_r is said to be the r th *left-definite space* associated with the pair $(\mathcal{H}, \mathbf{A})$.

It was proven in [49, Theorem 3.1] that $\mathcal{H}_r = (\mathcal{V}_r, \langle \cdot, \cdot \rangle_r)$ is also described as the left-definite space associated with the pair $(\mathcal{H}, \mathbf{A}^r)$, and we call \mathcal{H}_r the r th *left-definite space associated with the pair $(\mathcal{H}, \mathbf{A})$* . Specifically, we have:

- (1) \mathcal{H}_r is a Hilbert space,
- (2) $\mathcal{D}(\mathbf{A}^r)$ is a subspace of \mathcal{V}_r ,
- (3) $\mathcal{D}(\mathbf{A}^r)$ is dense in \mathcal{H}_r ,
- (4) $\langle x, x \rangle_r \geq k^r \langle x, x \rangle$ ($x \in \mathcal{V}_r$), and
- (5) $\langle x, y \rangle_r = \langle \mathbf{A}^r x, y \rangle$ ($x \in \mathcal{D}(\mathbf{A}^r)$, $y \in \mathcal{V}_r$).

The left-definite domains are defined as the domains of compositions of the self-adjoint operator \mathbf{A} , but the operator acting on this domain is slightly more difficult to define.

Definition 2.3.2. Let $\mathcal{H} = (\mathcal{V}, \langle \cdot, \cdot \rangle)$ be a Hilbert space. Suppose $\mathbf{A} : \mathcal{D}(\mathbf{A}) \subset \mathcal{H} \rightarrow \mathcal{H}$ is a self-adjoint operator that is bounded below by $k > 0$. Let $r > 0$. If there exists a self-adjoint operator $\mathbf{A}_r : \mathcal{H}_r \rightarrow \mathcal{H}_r$ that is a restriction of \mathbf{A} from the domain $\mathcal{D}(\mathbf{A})$ to $\mathcal{D}(\mathbf{A}^r)$, we call such an operator an r th *left-definite operator associated with $(\mathcal{H}, \mathbf{A})$* .

The connection between the r th left-definite operator and the r th composition of the self-adjoint operator \mathbf{A} is now made explicit.

Corollary 2.3.3 ([49, Corollary 3.3]). *Suppose \mathbf{A} is a self-adjoint operator in the Hilbert space \mathcal{H} that is bounded below by $k > 0$. For each $r > 0$, let $\mathcal{H}_r = (\mathcal{V}_r, \langle \cdot, \cdot \rangle_r)$ and*

\mathbf{A}_r denote, respectively, the r th left-definite space and the r th left definite operator associated with $(\mathcal{H}, \mathbf{A})$. Then

$$(1) \mathcal{D}(\mathbf{A}^r) = \mathcal{V}_{2r}, \text{ in particular, } \mathcal{D}(\mathbf{A}^{1/2}) = \mathcal{V}_1 \text{ and } \mathcal{D}(\mathbf{A}) = \mathcal{V}_2;$$

$$(2) \mathcal{D}(\mathbf{A}_r) = \mathcal{D}(\mathbf{A}^{(r+2)/2}), \text{ in particular, } \mathcal{D}(\mathbf{A}_1) = \mathcal{D}(\mathbf{A}^{3/2}) \text{ and } \mathcal{D}(\mathbf{A}_2) = \mathcal{D}(\mathbf{A}^2).$$

The left-definite theory is particularly important for self-adjoint differential operators that are bounded below, as they are generally unbounded. The theory is trivial for bounded operators, as shown in [49, Theorem 3.4].

Our applications of left-definite theory will be focused on differential operators which possess a complete orthogonal set of eigenfunctions in \mathcal{H} . In [49, Theorem 3.6] it was shown that the point spectrum of \mathbf{A} coincides with that of \mathbf{A}_r , and similarly for the continuous spectrum and for the resolvent set. It is possible to say more, a complete set of orthogonal eigenfunctions will persist throughout each space in the Hilbert scale.

Theorem 2.3.4 ([49, Theorem 3.7]). *If $\{\varphi_n\}_{n=0}^\infty$ is a complete orthogonal set of eigenfunctions of \mathbf{A} in \mathcal{H} , then for each $r > 0$, $\{\varphi_n\}_{n=0}^\infty$ is a complete set of orthogonal eigenfunctions of the r th left-definite operator \mathbf{A}_r in the r th left-definite space \mathcal{H}_r .*

Another perspective on the last theorem is that it gives us a valuable indicator for when a space is a left-definite space for a specific operator.

On the side we note that left-definite theory can be extended to bounded below operators by applying shifts. Uniqueness is then given up to the chosen shift.

A description of these left-definite spaces in terms of standard boundary conditions on a Hilbert space has been noticeably missing, despite the broad framework and range of results described above. This isn't to say that there are no descriptions of the left-definite spaces, just that they are not classically expressed by GKN theory.

Example. Let \mathbf{A} denote the usual self-adjoint operator with the Laguerre polynomials as a complete set of orthogonal eigenfunctions $\{\varphi_n\}_{n=0}^\infty$. For $\alpha > -1$ and

$j \in \mathbb{N}_0$, let $L_{\alpha+j}^2(0, \infty)$ be the Lebesgue space with norm induced by the inner product $\int_0^\infty f(t)\overline{g(t)}t^{\alpha+j}e^{-t}dt$. The n th left-definite Hilbert space associated with the pair $(\mathcal{H}, \mathbf{A}) = (L_\alpha^2(0, \infty), \mathbf{A})$, also possessing this complete set of eigenfunctions, is defined as $\mathcal{H}_n = (\mathcal{V}_n, \langle \cdot, \cdot \rangle_n)$, where

$$\mathcal{V}_n := \left\{ f : (0, \infty) \rightarrow \mathbb{C} \mid f \in \text{AC}_{\text{loc}}^{(n-1)}(0, \infty); f^{(n)} \in L_{\alpha+n}^2(0, \infty) \right\}$$

and

$$\langle p, q \rangle_n := \sum_{j=0}^n b_j(n, k) \int_0^\infty p^{(j)}(t)\overline{q^{(j)}(t)}t^{\alpha+j}e^{-t}dt \quad \text{for } (p, q \in \mathcal{P}),$$

where \mathcal{P} is the space of all (possibly complex-valued) polynomials. The constants $b_j(n, k)$ are defined as

$$b_j(n, k) := \sum_{i=0}^j \frac{(-1)^{i+j}}{j!} \binom{j}{i} (k+i)^n.$$

This description of a specific left-definite space is only included as a comparison to the simplicity of the results in Chapter 3, further details can be found in [49]. \spadesuit

2.4 Self-Adjoint Extensions of Symmetric Operators

There is a vast amount of literature concerning the extensions of symmetric operators. Here we present only that which pertains to self-adjoint extensions and applications to GKN theory. This will be primarily applied to linear differential operators.

Definition 2.4.1 (variation of [54, Section 14.2]). For a symmetric, closed operator \mathbf{A} on a Hilbert space \mathcal{H} , define the *positive defect space* and the *negative defect space*, respectively, by

$$\mathcal{D}_+ := \{f \in \mathcal{D}(\mathbf{A}^*) \mid \mathbf{A}^*f = if\} \quad \text{and} \quad \mathcal{D}_- := \{f \in \mathcal{D}(\mathbf{A}^*) \mid \mathbf{A}^*f = -if\}.$$

On the side we note that, in light of [19, Theorem XII.4.8], we can assume without loss of generality that all considered operators are closed because we are concerned exclusively with self-adjoint extensions of symmetric operators.

The dimensions $\dim(\mathcal{D}_+) = m_+$ and $\dim(\mathcal{D}_-) = m_-$, called the *positive* and *negative deficiency indices of \mathbf{A}* , respectively, are usually conveyed as the pair (m_+, m_-) . The deficiency indices of T correspond to how far from self-adjoint \mathbf{A} is. A symmetric operator \mathbf{A} has self-adjoint extensions if and only if its deficiency indices are equal [54, Section 14.8.8].

Theorem 2.4.2 ([54, Theorem 14.4.4]). *If \mathbf{A} is a closed, symmetric operator, then the subspaces $\mathcal{D}_{\mathbf{A}}$, \mathcal{D}_+ , and \mathcal{D}_- are linearly independent and their direct sum coincides with $\mathcal{D}_{\mathbf{A}^*}$, i.e.,*

$$\mathcal{D}_{\mathbf{A}^*} = \mathcal{D}_{\mathbf{A}} \dot{+} \mathcal{D}_+ \dot{+} \mathcal{D}_-.$$

(Here, subspaces $\mathcal{X}_1, \mathcal{X}_2, \dots, \mathcal{X}_p$ are said to be linearly independent, if $\sum_{i=1}^p x_i = 0$ for $x_i \in \mathcal{X}_i$ implies that all $x_i = 0$.)

Let $\ell[\cdot]$ be a Sturm–Liouville differential expression on some Hilbert space $L^2[(a, b), w]$ as in (2.2.2). Furthermore, let $\ell[\cdot]$ generate an expression $\ell^n[\cdot]$ of order $2n$ via composition, for $n \in \mathbb{N}$. The analysis of self-adjoint extensions does not involve changing the differential expression associated with the operator at all, merely the domain of definition, by applying boundary conditions.

Definition 2.4.3 ([54, Section 17.2]). The *maximal domain* of $\ell^n[\cdot]$ is given by

$$\mathcal{D}_{\max}^n = \mathcal{D}_{\max}(\ell^n) := \left\{ f : (a, b) \rightarrow \mathbb{C} \mid \begin{array}{l} f^{(k)}(x) \in \text{AC}_{\text{loc}}(a, b), \ k = 0, 1, \dots, 2n - 1; \\ f, \ell^n[f] \in L^2[(a, b), w] \end{array} \right\}.$$

The designation of “maximal” is appropriate in this case because $\mathcal{D}_{\max}(\ell^n)$ is the largest possible subspace for which ℓ^n maps back into $L^2[(a, b), w]$. For $f, g \in \mathcal{D}_{\max}(\ell^n)$ and $a < \alpha \leq \beta < b$ the *sesquilinear form* associated with ℓ^n by

$$[f, g]_n \Big|_{\alpha}^{\beta} := \int_{\alpha}^{\beta} \left\{ \ell^n[f(x)] \overline{g(x)} - \ell^n[\overline{g(x)}] f(x) \right\} w(x) dx. \quad (2.4.1)$$

The equation (2.4.1) is *Green’s formula* for $\ell^n[\cdot]$, and is an equivalent definition to the classical one from Sturm–Liouville theory utilizing Wronskians [52, Equation (3.5)].

Theorem 2.4.4 ([54, Section 17.2]). *The limits $[f, g]_n(b) := \lim_{x \rightarrow b^-} [f, g]_n|_\alpha^x$ and $[f, g]_n(a) := \lim_{x \rightarrow a^+} [f, g]_n|_x^\beta$ exist and are finite for $f, g \in \mathcal{D}_{\max}(\ell^n)$.*

Definition 2.4.5 ([54, Section 17.2]). The *minimal domain* of $\ell^n[\cdot]$ is given by

$$\mathcal{D}_{\min}^n = \mathcal{D}_{\min}(\ell^n) = \{f \in \mathcal{D}_{\max}(\ell^n) \mid [f, g]_n|_a^b = 0 \ \forall g \in \mathcal{D}_{\max}(\ell^n)\}.$$

The maximal and minimal operators associated with the expression $\ell^n[\cdot]$ are defined as $\mathbf{L}_{\min}^n = \{\ell^n, \mathcal{D}_{\min}^n\}$ and $\mathbf{L}_{\max}^n = \{\ell^n, \mathcal{D}_{\max}^n\}$ respectively. By [54, Section 17.2], these operators are adjoints of one another, i.e. $(\mathbf{L}_{\min}^n)^* = \mathbf{L}_{\max}^n$ and $(\mathbf{L}_{\max}^n)^* = \mathbf{L}_{\min}^n$.

In the context of differential operators, we work with the a special case of Theorem 2.4.2:

Theorem 2.4.6 ([54, Section 14.5]). *Let \mathcal{D}_{\max}^n and \mathcal{D}_{\min}^n be the maximal and minimal domains associated with the differential expression $\ell^n[\cdot]$, respectively. Then, for $n \in \mathbb{N}$,*

$$\mathcal{D}_{\max}^n = \mathcal{D}_{\min}^n \dot{+} \mathcal{D}_+^n \dot{+} \mathcal{D}_-^n. \quad (2.4.2)$$

Equation (2.4.2) is commonly known as *von Neumann's formula*. The symbol $\dot{+}$ denotes the direct sum, and $\mathcal{D}_+^n, \mathcal{D}_-^n$ are the defect spaces associated with the expression $\ell^n[\cdot]$. The decomposition can be made into an orthogonal direct sum by using the graph norm, see Section 3.1.2.

By [54, Section 14.8.8], if the operator \mathbf{L}_{\min}^n has any self-adjoint extensions, then the deficiency indices of \mathbf{L}_{\min}^n have the form (m, m) , where $0 \leq m \leq 2n$ and $2n$ is the order of $\ell^n[\cdot]$. Glazman [3, 30] has shown that the number m can take on any value between 0 and $2n$. In regards to differential expressions, the order of the operator is greater than or equal to each of the two deficiency indices by necessity. Hence, Sturm–Liouville expressions that generate self-adjoint operators have deficiency indices $(0, 0)$, $(1, 1)$ or $(2, 2)$. However, most of the applications in Chapter 3 require a complete

set of orthogonal eigenfunctions so choices are even more limited. Indeed, when these orthogonal eigenfunctions are assumed to be polynomial the Bochner classification [10] tells us that, up to a complex linear change of variable, the only such operators are Jacobi, Hermite, Laguerre and Bessel.

The discussion from Subsection 2.2.1 is now continued. If a differential expression is either in the limit circle case or regular at the endpoint a , it requires a boundary condition at a . If it is in the limit point case at the endpoint a , it does not require a boundary condition. The analogous statements are true at the endpoint b . These facts can be summed up in the following result.

Theorem 2.4.7. *Let $\mathbf{L}_{\min} = \{\ell, \mathcal{D}_{\min}\}$, where ℓ is a singular Sturm–Liouville differential expression.*

$$m_{\pm}(\mathbf{L}_{\min}) = \begin{cases} 2 & \text{if } \ell \text{ is l.c.c. at } a \text{ and } b, \\ 1 & \text{if } \ell \text{ is l.c.c. at } a \text{ and l.p.c. at } b \text{ or vice versa,} \\ 0 & \text{if } \ell \text{ is l.p.c. at } a \text{ and } b. \end{cases}$$

Sturm–Liouville differential expressions are extremely well-researched, see e.g. [8, 21] for an encyclopedic reference, so the deficiency indices are well-known in each of the cases of interest. Jacobi operators have deficiency indices $(2, 2)$, Laguerre have $(1, 1)$ and Hermite have $(0, 0)$. Bessel functions, on the other hand, are not complete in the relevant weighted L^2 space so are not considered here. Jacobi operators are in the limit circle case at both -1 and 1 (for α, β both in $[0, 1)$), Laguerre operators are in the limit circle case at 0 and the limit point case at ∞ (for $\alpha \in [0, 1)$), and Hermite operators are in the limit point case at both $\pm\infty$. Hermite operators are thus essentially self-adjoint and require no boundary conditions, so they are only mentioned in passing. The techniques developed in Chapter 3 apply trivially at endpoints which are in the limit point case. Regular endpoints are somewhat easier, and the spectrum associated with such operators are easily described by Perturbation Theory, see [61].

2.4.1 Glazman–Krein–Naimark (GKN) Theory

In order to formulate the GKN theorems, we recall an extension of linear independence to one that mods out by a subspace. This subspace will be the minimal domain in applications. The next two theorems form the core of GKN theory.

Definition 2.4.8 ([54, Section 14.6]). Let \mathcal{X}_1 and \mathcal{X}_2 be subspaces of a vector space \mathcal{X} such that $\mathcal{X}_1 \leq \mathcal{X}_2$. Let $\{x_1, x_2, \dots, x_r\} \subseteq \mathcal{X}_2$. We say that $\{x_1, x_2, \dots, x_r\}$ is *linearly independent modulo \mathcal{X}_1* if

$$\sum_{i=1}^r \alpha_i x_i \in \mathcal{X}_1 \text{ implies } \alpha_i = 0 \text{ for all } i = 1, 2, \dots, r.$$

Theorem 2.4.9 (GKN1, [54, Theorem 18.1.4]). Let $\mathbf{L}^n = \{\ell^n, \mathcal{D}_{\mathbf{L}}^n\}$ be a self-adjoint extension of the minimal operator $\mathbf{L}_{\min}^n = \{\ell^n, \mathcal{D}_{\min}^n\}$ with deficiency indices (m, m) . Then the domain $\mathcal{D}_{\mathbf{L}}^n$ consists of the set of all functions $f \in \mathcal{D}_{\max}^n$, which satisfy the conditions

$$[f, w_k]_n \Big|_a^b = 0, \quad k = 1, 2, \dots, m, \quad (2.4.3)$$

where $w_1, \dots, w_m \in \mathcal{D}_{\max}^n$ are linearly independent modulo \mathcal{D}_{\min}^n for which the relations

$$[w_j, w_k]_n \Big|_a^b = 0, \quad j, k = 1, 2, \dots, m \quad (2.4.4)$$

hold.

The requirements in equation (2.4.4) are commonly referred to as *Glazman symmetry conditions*. The converse of the GKN1 Theorem is also true.

Theorem 2.4.10 (GKN2, [54, Theorem 18.1.4]). Assume we are given arbitrary functions $w_1, w_2, \dots, w_m \in \mathcal{D}_{\max}^n$ which are linearly independent modulo \mathcal{D}_{\min}^n and which satisfy the relations (2.4.4). Then the set of all functions $f \in \mathcal{D}_{\max}^n$ which satisfy the conditions (2.4.3) is domain of a self-adjoint extension of \mathbf{L}_{\min}^n .

These two theorems completely answer the question of how boundary conditions can be used to create self-adjoint extensions. Applications of this theory hinge

on determining the proper w_k 's that will define the domain of the desired self-adjoint extension. More intuition for how these vectors that are linearly independent modulo the minimal domain are creating self-adjoint extensions can be found in unitary matrices.

Theorem 2.4.11 ([54, Theorem 18.1.2]). *Every self-adjoint extension L of the operator L_{\min}^n with the deficiency indices (m, m) can be characterized by means of a unitary $m \times m$ matrix $u = [u_{jk}]$ in the following way:*

Its domain of definition \mathcal{D}_L is the set of all functions $f(x)$ of the form

$$f(x) = y(x) + \psi(x),$$

where $y(x) \in \mathcal{D}_{\min}^n$. Let φ_j be a basis vector of \mathcal{D}_+ . Then $\psi(x)$ can be written as the linear combination:

$$\psi(x) = \varphi_j(x) + \sum_{k=1}^m u_{kj} \overline{\varphi_k(x)}, \quad j = 1, \dots, m.$$

Conversely, every unitary $m \times m$ matrix $u = [u_{jk}]$ determines in the way described above a certain self-adjoint extension L of the operator L_{\min}^n . The correspondence thus established between L and u is one-to-one.

Hence, the w_1, \dots, w_m functions in the GKN1 Theorem are represented as the sum from at least one function in each of \mathcal{D}_+ and \mathcal{D}_- , as the unitary matrix describing the extension must have full rank. Full statements and proofs of the last three theorems can be found in [54].

2.5 Anderson-type Hamiltonians

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space, and consider the sequence of independent random complex variables $X_n(w), w \in \Omega$. We explain a simple application of Kolmogorov's 0-1 Law to Anderson-type Hamiltonians using the standard probabilistic setup described in [37] (also see [1]), where the reader can find all the necessary definitions and basic properties.

Assume that $\Omega = \prod_{n=0}^{\infty} \Omega_n$, where Ω_n are different probability spaces, $w = (w_1, w_2, \dots)$, $w_n \in \Omega_n$ and the probability measure on Ω is introduced as the product measure of the corresponding measures on Ω_n . Each of the independent random variables $X_n(w)$ depends only on the n -th coordinate, w_n , of w .

It is a standard observation that any sequence of independent random variables on an abstract probability space is similar to such a sequence X_n defined, for instance, on an infinite dimensional torus. Hence, without loss of generality we have $\Omega = \prod_{n=0}^{\infty} \Omega_n$, where each Ω_n is a copy of the unit circle with normalized Lebesgue measure, see e.g. [37] (where the unit interval was used instead of \mathbb{T}).

It is well-known that the properties we are interested in (cyclicity, spectral properties, etc.) are in fact an event. Explicitly, the set A of w , such that the function corresponding to the sequence $\{X_n(w)\}$ satisfies the desired property, is measurable: $A \in \mathcal{A}$. We will be mostly interested in the events A that do not depend on the values of any finite number of variables X_n , i.e. the sets $A \in \mathcal{A}$ with the property that if $w \in A$ and $X_n(w) = X_n(w')$ for all but finitely many n then $w' \in A$. *Kolmogorov's 0-1 Law* states that the probability of any such event is 0 or 1.

Now, consider a self-adjoint operator H on a separable Hilbert space \mathcal{H} and a sequence $\{\varphi_n\} \subset \mathcal{H}$ of linearly independent unit vectors. Let $\omega = (\omega_1, \omega_2, \dots)$ be a random variable corresponding to a probability measure \mathbb{P} on \mathbb{R}^{∞} that satisfies Kolmogorov's 0-1 Law. In particular, the parameters ω_n are chosen i.i.d. (independent, identically distributed) with respect to \mathbb{P} .

An *Anderson-type Hamiltonian* [34] is an almost surely self-adjoint operator associated with the formal expression

$$H_{\omega} = H + V_{\omega} \quad \text{on } \mathcal{H}, \quad V_{\omega} = \sum_n \omega_n \langle \cdot, \varphi_n \rangle \varphi_n. \quad (2.5.1)$$

As is customary, assume that the vectors φ_n be orthogonal. However, many properties readily extend to the case of non-orthogonal φ_n so long as (2.5.1) almost surely defines a self-adjoint operator.

Observation 2.5.1 (Kolmogorov's 0-1 law applied to Anderson-type Hamiltonians). *Consider the Anderson-type Hamiltonian H_ω given by (2.5.1). Assume that the probability distribution \mathbb{P} satisfies the 0-1 law. Then those spectral properties that are invariant under finite rank perturbations are enjoyed by H_ω almost surely or almost never.*

The archetype Anderson-type Hamiltonian is the discrete Schrödinger operator with random potential on $l^2(\mathbb{Z}^d)$, given by

$$Hf(x) = -\Delta f(x) = -\sum_{|n|=1} (f(x+n) - f(x)), \quad \varphi_n(x) = \delta_n(x) = \begin{cases} 1 & x = n, \\ 0 & \text{else.} \end{cases} \quad (2.5.2)$$

This operator is often used to model quantum mechanical phenomena in a crystalline structure with random on-site potentials, and appears in many fields of mathematics. With regards to perturbation theory, one of the main challenges in approaching Anderson-type Hamiltonians is that they feature an almost surely non-compact perturbation. It is apparent by the survey of results in Subsection 2.1, classical perturbation theory is at a loss at how to handle this scenario.

CHAPTER THREE

Boundary Conditions associated with Left-Definite Theory

A wide variety of literature concerns the study of left-definite theory applied to Sturm–Liouville differential operators. The interest arises primarily from the groundbreaking paper of Littlejohn and Wellman [49]. The paper describes the creation of a continuum of left-definite spaces and left-definite operators associated with an arbitrary self-adjoint operator that is bounded below by a positive constant in a Hilbert space. Prior to [49], research had been conducted only in the “first” left-definite setting. This theory has been applied to many types of self-adjoint differential operators, including those stemming from the second-order differential equations of Hermite, Legendre, Jacobi, Laguerre, and Fourier. Excellent surveys of these results are [12] and [50].

The paper of Littlejohn and Wellman [49] managed to characterize these left-definite spaces in terms of other Hilbert spaces defined with integral operators. A key point of left-definite theory is that each left-definite space will be nested and dense within the original Hilbert space. However, some critics felt somewhat uneasy with the fact that the left-definite spaces (in their opinions) lack an explicit mention of boundary conditions.

One of the goals of this paper is to address these concerns. We present classical boundary conditions that exist for self-adjoint differential operators which possess a complete system of orthogonal eigenfunctions. These boundary conditions are formulated in terms of Glazman–Krein–Naimark (from now on abbreviated by GKN) theory, which entirely describes self-adjoint extensions for a closed, symmetric operator with equal deficiency indices.

This framework allows for the construction of the boundary conditions for the left-definite spaces of the classical Legendre differential operator explicitly. Previous work using GKN conditions to describe the left-definite domains is limited to very recent progress by Littlejohn and Wicks [51, 52]. The results concern the classical Legendre differential operator exclusively and give GKN conditions describing the fourth left-definite domain, which is associated with the square of the differential operator, L^2 , or the case where $n = 2$ below. Additionally, Littlejohn and Wicks formulate their results in terms of “separated” boundary conditions, whereas “coupled” boundary conditions are used throughout this paper. This is a matter of preference, but using coupled boundary conditions simplifies calculations considerably, as they are easier to access via the sesquilinear form dealt with by GKN theory.

In this work we introduce a systematic approach, which reduces the amount of cumbersome computations in this field. This perspective enables us to harvest the finite dimensional nature of defect spaces. An alternative approach to this problem is through Sturm–Liouville theory, e.g. [27, 39], but the literature focuses on the first left-definite theory and does not produce GKN conditions.

The interest in differential operators which possess a complete system of orthogonal eigenfunctions originates with Theorem 2.3.4 [49] that says this same system will be present in each of the different left-definite domains. Hence, there is an indicator for when a self-adjoint extension is a left-definite domain, and this simplifies the process. A second-order linear differential equation satisfied by a complete orthogonal system of polynomials with absolutely continuous measures of orthogonality has a second linearly independent solution [33, Section 3.6]. This second linearly independent solution is often called a function of the second kind, and their existence plays an essential role in our examples.

The Legendre differential operator example is particularly important because there are essentially only four Sturm–Liouville operators with a complete set of or-

thogonal eigenfunctions. The Bochner classification [10] tells us that, up to a complex linear change of variable, the only such operators with polynomial eigenfunctions are Jacobi, Hermite, Laguerre and Bessel. Of these, the Jacobi differential expressions require the most boundary conditions. The Legendre expression is a special case of Jacobi that has an immense amount of literature, so it was ideal for such an exploration of GKN conditions with respect to left-definite theory. The framework of Section 3.2 both extends to other Jacobi differential expressions (other values of the parameters α and β), and reduces to cover the cases of Hermite, Laguerre and Bessel. The broader concepts of Section 3.4 are expressed with this in mind as well.

While our applications to the classical systems use polynomial eigenfunctions, a keen reader may observe that our general results consider systems of eigenfunctions, which are not necessarily polynomials. This general approach suggests other open problems: What adjustments are necessary when the self-adjoint operator has a spectrum that is not discrete? That is, given some non-standard extension of a differential operator, can we describe the corresponding left-definite domain? How about the left-definite domain for compositions of the operator?

The approaches and ideas used in our three distinct types of results in Sections 3.2 through 3.4 differ vastly from one another. As a consequence, the setup changes slightly from one section to another.

In Section 3.1 we construct a systematic framework around the method of finding GKN conditions that make differential expressions into self-adjoint differential operators. We show that eigenfunctions of a self-adjoint operator, which are linearly independent modulo the minimal domain, yield GKN conditions for the operator. Subsection 3.1.2 describes the graph norm that can be endowed on a Hilbert space and justifies intuition about the decomposition of the maximal domain.

In Section 3.2, explicit self-adjoint extensions are given by showing that eigenfunctions themselves lead to suitable GKN conditions for powers \mathbf{L}^n of the classical

Legendre operator \mathbf{L} . The case $n = 2$ was the topic of [51]. One of the key features of our approach is that it utilizes the functions of the second kind. In examples, we prove that the first n eigenfunctions work for \mathbf{L}^n for $n = 2, \dots, 5$. The statement has been verified numerically for $n \leq 16$ due to the special structure of the matrix of sesquilinear forms discussed in Subsection 3.2.1. We show a necessary condition for eigenfunctions and functions of the second kind to be suitable “test” functions for linear independence modulo the minimal domain in Subsection 3.2.2. The sufficiency of this condition is discussed and conjectured.

Motivated by the Legendre example, it is shown in Section 3.3 that for left-definite operators with pure point spectrum (only eigenvalues) there exist eigenfunctions (corresponding to some eigenvalues) that generate GKN conditions. The method of proof for this result differs from the explicit computations that were used in the Legendre example. It relies on working with the graph norm. We believe this to be the first general result in this direction. The idea is to reduce the problem to its essence: finite dimensional linear algebra. This is accomplished by using the fact that the defect spaces and minimal domain are orthogonal with respect to graph norm, and properties of the eigenfunctions.

In Section 3.4 the goal is to determine which boundary conditions describe left-definite domains. This question is then explored by comparing the left-definite domains for these differential operators with the complete system of orthogonal polynomials and their GKN conditions to boundary conditions that stem from the definition of the Sturm–Liouville operator. The work improves and simplifies a proof of a fact from [52]. The central conjecture stating the equivalence of the following four sets is still partially open:

- The n th left definite domain.
- The maximal domain with GKN conditions determined by the first m orthogonal polynomials. (Here, m denotes the deficiency indices.)

- The maximal domain with GKN conditions determined by any m orthogonal polynomials.
- The maximal domain with certain explicit boundary conditions.

Other ramifications and specific discussions of individual systems of orthogonal polynomials and their differential equations follows.

3.1 *Eigenfunctions as GKN Conditions*

The Glazman–Krein–Naimark construction of self-adjoint extensions of symmetric operators, detailed in Subsection 2.4.1, is analyzed to determine which extension coincides with the left-definite space associated to differential operators whose domains possess a complete set of orthogonal eigenfunctions. The most promising choices of these GKN boundary conditions will be these eigenfunctions themselves. However, all choices of GKN boundary conditions rely on functions that are linearly independent modulo the minimal domain so we begin with a comprehensive discussion of this idea.

3.1.1 *Linear Independence Modulo the Minimal Domain*

Consider a symmetric expression ℓ with deficiency indices (m, m) on the Hilbert space $L^2[(a, b), w]$. The following simple result will be used to test for linear independence modulo \mathcal{D}_{\min} . The main idea is to find a sufficient condition in terms of a certain matrix of sesquilinear forms (corresponding to ℓ) having full rank.

Proposition 3.1.1. *Given vectors $w_1, \dots, w_r \in \mathcal{D}_{\max}$, $r \leq 2m$. Assume that the $r \times r$ matrix \mathbf{M} with entries $\mathbf{M}_{ik} = [w_i, w_k]_a^b$ for $1 \leq i, k \leq r$ has full rank. Then w_1, \dots, w_r are linearly independent modulo \mathcal{D}_{\min} .*

We will prove this proposition in a moment.

In virtue of Linear Algebra (dimension counting, and realizing that removing vectors from a basis leaves behind a linearly independent set) we obtain an immediate consequence, which both Subsection 3.1.3 and Section 3.2 rely heavily on.

Corollary 3.1.2. *Given vectors $w_1, \dots, w_r \in \mathcal{D}_{\max}$, $r \leq 2m$. Assume that for some vectors $w_{r+1}, \dots, w_s \in \mathcal{D}_{\max}$, $r \leq s \leq 2m$, the $s \times s$ matrix \mathbf{M} with entries $\mathbf{M}_{ik} = [w_i, w_k]_a^b$ (for $1 \leq i, k \leq s$) has full rank. Then w_1, \dots, w_s are linearly independent modulo \mathcal{D}_{\min} , and so are the vectors w_1, \dots, w_r .*

Remark. In our applications below, we usually have $r = m$ and $s = 2m$. Moreover, w_1, \dots, w_m will be eigenfunctions, and w_{m+1}, \dots, w_{2m} will be functions of the second kind.

Proof of Proposition 3.1.1. Our goal is to show that the set w_1, \dots, w_r is linearly independent modulo the minimal domain \mathcal{D}_{\min} . To that end, suppose

$$\sum_{k=1}^r \alpha_k w_k \in \mathcal{D}_{\min}. \quad (3.1.1)$$

We want to show that $\alpha_k = 0$ for all $k = 1, \dots, r$.

The definition of the minimal domain says that $y \in \mathcal{D}_{\min}$ if and only if $[y, w]_a^b = 0$ for all $w \in \mathcal{D}_{\max}$. Letting $y = w_i$, $w = \sum_{k=1}^r \alpha_k w_k$ and using the linearity of the sesquilinear form, we see that (3.1.1) implies

$$\sum_{k=1}^r \alpha_k [w_i, w_k]_a^b = 0 \text{ for } i = 1, \dots, r. \quad (3.1.2)$$

Now, interpreting (3.1.2) for a specific i as the i th row of a matrix equation, we see that (3.1.2) is equivalent to the matrix equation

$$\mathbf{M}\alpha = \mathbf{0} \quad \text{with} \quad \mathbf{M} = \begin{pmatrix} [w_1, w_1]_a^b & \dots & [w_1, w_r]_a^b \\ \vdots & \ddots & \vdots \\ [w_r, w_1]_a^b & \dots & [w_r, w_r]_a^b \end{pmatrix}, \quad \alpha = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_r \end{pmatrix},$$

and the zero vector $\mathbf{0} \in \mathbb{R}^r$.

And since we assume that \mathbf{M} has full rank, we conclude that $\alpha_k = 0$ for all $k = 1, \dots, r$. \square

This result is not particularly surprising, yet adds to the formal framework surrounding the concept of linear independence modulo the minimal domain. In fact, the notion of two functions being orthogonal in a Hilbert space, i.e. their inner product is equal to 0, implies that they are linearly independent. Indeed, the creation of a matrix of inner products would imply a similar result regarding linear independence in the Hilbert space (where the converse is still false). However, this construction would not take into account the operator itself, or the different domains associated with it.

Recall that all functions in the maximal domain possess a decomposition via Theorem 2.4.6. The part corresponding to the minimal domain for these functions is destroyed when plugged in to the sesquilinear form. Hence, the sesquilinear form can be viewed as the annihilator of the minimal domain and is therefore the ideal tool available to assess whether functions are linearly independent modulo the minimal domain. The definition of the sesquilinear form in equation (2.4.1) as the difference of two inner products further reinforces this intuition.

3.1.2 The Graph Norm

Let \mathbf{A} be a densely defined symmetric operator on a separable Hilbert space \mathcal{H} . Furthermore, for $x, y \in \mathcal{D}(\mathbf{A}^*)$, denote the **graph inner product** by

$$\langle x, y \rangle_{\mathbf{A}} := \langle x, y \rangle_{\mathcal{H}} + \langle \mathbf{A}^* x, \mathbf{A}^* y \rangle_{\mathcal{H}}.$$

This section will use the convention that $\mathcal{D}(\mathbf{A}^*)$ has the topology defined by the **graph norm** $\|x\|_{\mathbf{A}} := \langle x, x \rangle_{\mathbf{A}}^{1/2}$ induced by the inner product $\langle x, y \rangle_{\mathbf{A}}$, unless the contrary is explicitly stated. The graph norm allows for some more elegant results in the theory of self-adjoint extensions, and will be central to our main theorems.

Lemma 3.1.3 ([19, Lemma XII.4.10]). *Using the above conventions, we have that:*

- (1) $\mathcal{D}(\mathbf{A})$, \mathcal{D}_+ , and \mathcal{D}_- are closed orthogonal subspaces of the Hilbert space $\mathcal{D}(\mathbf{A}^*)$.

(2) $\mathcal{D}(\mathbf{A}^*) = \mathcal{D}(\mathbf{A}) \oplus_{\mathbf{A}} \mathcal{D}_+ \oplus_{\mathbf{A}} \mathcal{D}_-$. Here $\oplus_{\mathbf{A}}$ denotes the orthogonal sum, with respect to the graph inner product.

The results in Section 3.3 heavily rely on this orthogonal decomposition so a proof of the Lemma, following that of [19], is included.

Proof. The space $\mathcal{D}(\overline{\mathbf{A}})$ is closed by the above note, while \mathcal{D}_+ and \mathcal{D}_- are closed because they are finite dimensional. Since \mathcal{D}_+ and \mathcal{D}_- are clearly linear subspaces of $\mathcal{D}(\mathbf{A}^*)$, it remains to show that the spaces $\mathcal{D}(\overline{\mathbf{A}})$, \mathcal{D}_+ , and \mathcal{D}_- are mutually orthogonal, and that their sum is $\mathcal{D}(\mathbf{A}^*)$.

Suppose $d \in \mathcal{D}(\overline{\mathbf{A}})$, $d_+ \in \mathcal{D}_+$, and $d_- \in \mathcal{D}_-$. We will show that $\langle d, d_+ \rangle_{\mathbf{A}} = \langle d, d_- \rangle_{\mathbf{A}} = \langle d_-, d_+ \rangle_{\mathbf{A}} = 0$. First, since $\mathbf{A}^* \supseteq \overline{\mathbf{A}}$ we compute

$$\begin{aligned} \langle d, d_+ \rangle_{\mathbf{A}} &= \langle d, d_+ \rangle + \langle \mathbf{A}^* d, \mathbf{A}^* d_+ \rangle = \langle d, d_+ \rangle + \langle \overline{\mathbf{A}} d, \mathbf{A}^* d_+ \rangle \\ &= \langle d, d_+ \rangle + \langle \overline{\mathbf{A}} d, id_+ \rangle = \langle d, d_+ \rangle + \langle d, i\overline{\mathbf{A}}^* d_+ \rangle \\ &= \langle d, d_+ \rangle + \langle d, i\mathbf{A}^* d_+ \rangle = \langle d, d_+ \rangle + \langle d, i^2 d_+ \rangle = 0. \end{aligned}$$

Similarly, $\langle d, d_- \rangle_{\mathbf{A}} = 0$. Next,

$$\begin{aligned} \langle d_-, d_+ \rangle_{\mathbf{A}} &= \langle d_-, d_+ \rangle + \langle \mathbf{A}^* d_-, \mathbf{A}^* d_+ \rangle \\ &= \langle d_-, d_+ \rangle + \langle -id_-, id_+ \rangle = 0. \end{aligned}$$

Hence the spaces $\mathcal{D}(\overline{\mathbf{A}})$, \mathcal{D}_+ , and \mathcal{D}_- are mutually orthogonal, and $\mathcal{D}(\overline{\mathbf{A}}) \oplus_{\mathbf{A}} \mathcal{D}_+ \oplus_{\mathbf{A}} \mathcal{D}_-$ is contained in $\mathcal{D}(\mathbf{A}^*)$.

To show that they are equal, we will show that zero is the only vector orthogonal to the three subspaces involved. Suppose v is orthogonal to $\mathcal{D}(\overline{\mathbf{A}})$, \mathcal{D}_+ , and \mathcal{D}_- . Then $0 = \langle d, v \rangle_{\mathbf{A}} = \langle d, v \rangle + \langle \mathbf{A}^* d, \mathbf{A}^* v \rangle$, for all d in $\mathcal{D}(\overline{\mathbf{A}})$. Hence $\langle d, v \rangle = -\langle \mathbf{A}^* d, \mathbf{A}^* v \rangle = -\langle \mathbf{A} d, \mathbf{A}^* v \rangle$ because \mathbf{A} is symmetric and so $\mathbf{A} = \mathbf{A}^*$ on $\mathcal{D}(\overline{\mathbf{A}})$.

Recall that $\langle \cdot, v \rangle$ is a continuous linear functional on the dense subset $\mathcal{D}(\overline{\mathbf{A}})$ of the original Hilbert space \mathcal{H} . By the definition of the adjoint, we see that $\mathbf{A}^* v$ is in

$\mathcal{D}(\mathbf{A}^*)$ and so $\mathbf{A}^*(\mathbf{A}^*v) = -v$. Hence, we have $(I + \mathbf{A}^*\mathbf{A}^*)v = (I + i\mathbf{A}^*)(I - i\mathbf{A}^*)v = 0$. And so we obtain $\mathbf{A}^*[(I - i\mathbf{A}^*)v] = i(I - i\mathbf{A}^*)v$, or $(I - i\mathbf{A}^*)v \in \mathcal{D}_+$. Also, if $d_+ \in \mathcal{D}_+$, then

$$\begin{aligned} 0 &= \langle v, d_+ \rangle_{\mathbf{A}} = \langle v, d_+ \rangle + \langle \mathbf{A}^*v, \mathbf{A}^*d_+ \rangle = \langle v, d_+ \rangle + \langle \mathbf{A}^*v, id_+ \rangle \\ &= \langle v, d_+ \rangle - i\langle \mathbf{A}^*v, d_+ \rangle = \langle (I - i\mathbf{A}^*)v, d_+ \rangle. \end{aligned}$$

Since $(I - i\mathbf{A}^*)v$ is in \mathcal{D}_+ , this implies that $(I - i\mathbf{A}^*)v = 0$. Hence $\mathbf{A}^*v = -iv$, or $v \in \mathcal{D}_-$. But $\langle \mathcal{D}_-, v \rangle_{\mathbf{A}} = 0$. Hence $v = 0$. Therefore $\mathcal{D}(\mathbf{A}^*) = \mathcal{D}(\overline{\mathbf{A}}) \oplus_{\mathbf{A}} \mathcal{D}_+ \oplus_{\mathbf{A}} \mathcal{D}_-$. \square

The previous lemma can be viewed with regards to differential operators by using that the maximal and minimal operators are adjoints of one another. Our differential operators are assumed to be closed, so it is possible to replace $\mathcal{D}(\mathbf{A})$ with \mathcal{D}_{\min} and $\mathcal{D}(\mathbf{A}^*)$ with \mathcal{D}_{\max} , while still assuming that \mathcal{D}_{\max} is endowed with the graph norm. Hence, the lemma translates into von Neumann's formula (2.4.2), but the decomposition is orthogonal due to the different norm. The $r/2$ graph norm of \mathbf{A} will be of particular interest, and is denoted by $\langle x, y \rangle_{\mathbf{A}^{r/2}} = \langle x, y \rangle_{\mathcal{H}} + \langle \mathbf{A}^{r/2}x, \mathbf{A}^{r/2}y \rangle_{\mathcal{H}}$. The operator \mathbf{A} is assumed to be self-adjoint and bounded below by $k > 0$, as in Section 2.3.

Lemma 3.1.4. *The r th left-definite norm is equivalent to the $r/2$ graph norm. Concretely,*

$$\|x\|_r^2 \leq \|x\|_{\mathbf{A}^{r/2}}^2 \leq C\|x\|_r^2 \quad \text{for } x \in \mathcal{D}(\mathbf{A}^{r/2}),$$

where the constant C depends on k and r .

Proof. The r th left-definite inner product can be defined via Definition 2.3.1 as $\|x\|_r^2 = \langle x, x \rangle_r = \langle \mathbf{A}^{r/2}x, \mathbf{A}^{r/2}x \rangle_{\mathcal{H}}$. Also, recall that the definition of the r th left-definite space implied the stipulation $\langle x, x \rangle_r \geq k^r \langle x, x \rangle_{\mathcal{H}}$. Then,

$$\|x\|_{\mathbf{A}^{r/2}}^2 = \langle \mathbf{A}^{r/2}x, \mathbf{A}^{r/2}x \rangle_{\mathcal{H}} + \langle x, x \rangle_{\mathcal{H}} = \|x\|_r^2 + \|x\|_{\mathcal{H}}^2 \geq \|x\|_r^2,$$

and

$$\begin{aligned}
||x||_r^2 &= \frac{1}{2}\langle x, x \rangle_r + \frac{1}{2}\langle x, x \rangle_r \\
&\geq \frac{k^r}{2}\langle x, x \rangle_{\mathcal{H}} + \frac{1}{2}\langle x, x \rangle_r \\
&= \frac{1}{2} [k^r \langle x, x \rangle_{\mathcal{H}} + \langle \mathbf{A}^{r/2} x, \mathbf{A}^{r/2} x \rangle_{\mathcal{H}}] \\
&\geq \frac{1}{2} \min\{k^r, 1\} ||x||_{\mathbf{A}^{r/2}}^2.
\end{aligned}$$

Furthermore, no problems arise by passing to the $r/2$ graph norm instead of the usual r graph norm. This is because the domain of the $r/2$ graph norm coincides with the $r/2$ th left-definite space and $\mathcal{D}(\mathbf{A}_{r/2}) \supset \mathcal{D}(\mathbf{A}_r)$. We conclude that the two norms are indeed equivalent. \square

3.1.3 The Matrix of Sesquilinear Forms

Consider a symmetric expression ℓ with deficiency indices (m, m) on the Hilbert space $L^2[(a, b), w]$. Let $\mathbf{L} = \{\ell, \mathcal{D}_{\mathbf{L}}\}$ be a self-adjoint extension. Assume that the domain of \mathbf{L} includes a complete set of orthogonal eigenfunctions, say $\{P_k\}_{k=0}^{\infty}$. The GKN1 Theorem (Theorem 2.4.9) states that all self-adjoint extensions are obtained by imposing m GKN conditions on the maximal domain. GKN conditions are induced by functions w_1, \dots, w_m , which satisfy three conditions:

- (C1) The functions w_1, \dots, w_m must be linearly independent modulo the minimal domain.
- (C2) The complete system of orthogonal eigenfunctions must be included in the domain, pursuant to equation (2.4.3).
- (C3) The functions w_1, \dots, w_m must satisfy the Glazman symmetry conditions in equation (2.4.4).

Later we will choose w_1, \dots, w_m to be eigenfunctions. In that case, the first item (C1) implies both (C2) and (C3).

Remark 3.1.5. In fact, item (C3) can in general be obtained from (C1), if we allow for an insignificant modification of the w_1, \dots, w_m . Indeed, the Glazman symmetry conditions (C3) are easily attained by taking linear combinations of vectors satisfying (C1) via a procedure that is similar to the Gram–Schmidt orthogonalization, using the sesquilinear form instead of an inner product. We notice that such linear combinations will not change (C1). They will span the same domain modulo \mathcal{D}_{\min} . So they will also not change property (C2).

By assumption we have $\dim(\mathcal{D}_+ \dot{+} \mathcal{D}_-) = 2m$. A basis of this space mod (\mathcal{D}_{\min}) would be ideal. But, if w_1, \dots, w_m are linearly independent modulo the minimal domain, then they can be completed to a basis w_1, \dots, w_{2m} ; and vice versa.

Consider the matrix

$$\mathbf{M} = \left(\begin{array}{ccc|ccc} [w_1, w_1] & \dots & [w_1, w_m] & [w_1, w_{m+1}] & \dots & [w_1, w_{2m}] \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ [w_m, w_1] & \dots & [w_m, w_m] & [w_m, w_{m+1}] & \dots & [w_m, w_{2m}] \\ \hline [w_{m+1}, w_1] & \dots & [w_{m+1}, w_m] & [w_{m+1}, w_{m+1}] & \dots & [w_{m+1}, w_{2m}] \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ [w_{2m}, w_1] & \dots & [w_{2m}, w_m] & [w_{2m}, w_{m+1}] & \dots & [w_{2m}, w_{2m}] \end{array} \right), \quad (3.1.3)$$

where each sesquilinear form is evaluated from a to b .

We formulate sufficient conditions under which eigenfunctions act as GKN conditions. Though the set up seems less natural, the result will be shown to bear useful consequences. The theorem shows that, under the assumption that eigenfunctions $\{P_{k_i}\}_{i=1}^m$ can be completed to a basis of $\mathcal{D}_+ \dot{+} \mathcal{D}_-$, these eigenfunctions are then appropriate GKN conditions.

Theorem 3.1.6. Let $\mathbf{L} = \{\ell, \mathcal{D}_{\mathbf{L}}\}$ be a self-adjoint operator on the Hilbert space $L^2[(a, b), w]$, and be an extension of a minimal symmetric operator that has deficiency

indices (m, m) . Assume that $\mathcal{D}_{\mathbf{L}}$ includes a complete set of orthogonal eigenfunctions, $\{P_k\}_{k=0}^{\infty}$. Furthermore, assume that a basis modulo \mathcal{D}_{\min} of the defect spaces $\mathcal{D}_+ \dot{+} \mathcal{D}_-$ is given by the collection $\{P_{k_1}, \dots, P_{k_m}, f_1, \dots, f_m\}$. Then $\mathcal{D}_{\mathbf{L}}$ is given by imposing $\{P_{k_1}, \dots, P_{k_m}\}$ as GKN conditions on \mathcal{D}_{\max} .

Before we prove this result, we take an excursion via two corollaries. In combination with Corollary 3.1.2, a slight modification of the proof of Theorem 3.1.6 immediately yields a similar result for general w_1, \dots, w_{2m} .

Corollary 3.1.7. Consider a symmetric operator with expression ℓ on $L^2[(a, b), w]$ that has deficiency indices (m, m) . If \mathbf{M} defined as in equation (3.1.3) has full rank for some choice of $w_1, \dots, w_{2m} \in \mathcal{D}_{\max}(\ell)$, then any subset of m of these induces GKN conditions so long as we drop the symmetry condition (C3).

In Corollary 3.1.7, we do not claim that these conditions induce a particular self-adjoint extension, but rather just one of the infinitely many possible ones, again, not expecting the GKN symmetry condition (C3). In the next section, we will apply another immediate consequence of the Theorem to powers of a self-adjoint extension associated with the Legendre expression. Assuming that \mathbf{L} is bounded below, we can consider the self-adjoint operator (associated with the differential expression ℓ^n) that arises from the $2n$ th left-definite domain for \mathbf{L} . Consider the matrix \mathbf{M}_{nm} where the sesquilinear forms $[\cdot, \cdot]$ are the ones corresponding to ℓ^n , which we generally denote by $[\cdot, \cdot]_n$.

Corollary 3.1.8. Assume that nm of the w_1, \dots, w_{2nm} functions are eigenfunctions (e.g. $w_k = P_k$ for $k = 1, \dots, nm$). If the corresponding $(2nm) \times (2nm)$ matrix \mathbf{M} from equation (3.1.3) has full rank, then the domain of the $2n$ th left-definite operator can be represented by imposing GKN conditions with those eigenfunctions on the maximal domain.

Examples in Section 3.2 show that, for small values of n , the first m eigenfunctions can in fact serve as half of these basis vectors. Therefore, they can be used to form GKN conditions.

In accordance with equation (3.1.4) below, orthogonal functions which also satisfy the eigenvalue equation, are automatically symmetric in the sense of Glazman's condition (C3). So, the entire problem of imposing appropriate GKN conditions on symmetric operators to yield left-definite self-adjoint extensions is reduced to showing that the upper-right quadrant of the matrix \mathbf{M} has full rank. We explore this further below in Proposition 3.2.2 for Legendre, and the remark following the proof of Proposition 3.2.2 for more general settings.

Proof of Theorem 3.1.6. The collection $\{P_{k_1}, \dots, P_{k_m}, f_1, \dots, f_m\}$ forms a basis of $\mathcal{D}_+ \dot{+} \mathcal{D}_-$, so all self-adjoint extensions of the minimal operator come from using m distinct GKN conditions written as:

$$G_i = a_{i,1}P_{k_1} + a_{i,2}P_{k_2} + \dots + a_{i,m}P_{k_m} + a_{i,m+1}f_1 + a_{i,m+2}f_2 + \dots + a_{i,2m}f_m,$$

for $i = 1, \dots, m$. The GKN1 Theorem 2.4.9 implies that

$$\mathcal{D}_{\mathbf{L}} = \{f \in \mathcal{D}_{\max} \mid [f, G_i]_a^b = 0, \ i = 1, \dots, m \text{ for some choice of } a_{i,j} \text{'s}\}.$$

The claim is then that $a_{i,j} = 0$ for all $j > m$. In particular, this choice of constants $a_{i,j}$'s needs to include the subset of orthogonal eigenfunctions $\{P_{k_1}, \dots, P_{k_m}\}$ in the domain. Notice that an application of Green's formula for the sesquilinear form yields

$$[P_i, P_j]_a^b = \int_a^b \ell[P_i]P_j w dx - \int_a^b P_i \ell[P_j] w dx = (\lambda_i - \lambda_j) \int_a^b P_i P_j w dx = 0. \quad (3.1.4)$$

Here, if $i = j$ then $\lambda_i - \lambda_j = 0$, and if $i \neq j$ then we use the orthogonality of P_i and P_j .

The Glazman symmetry conditions (C3) follow immediately.

Fix the index i and test the chosen G_i against these orthogonal eigenfunctions in the sesquilinear form as follows:

$$\begin{aligned}
0 &= [P_{k_1}, G_i]_a^b = 0 + \cdots + 0 + a_{i,m+1}[P_{k_1}, f_1]_a^b + \cdots + a_{i,2m}[P_{k_1}, f_m]_a^b, \\
0 &= [P_{k_2}, G_i]_a^b = 0 + \cdots + 0 + a_{i,m+1}[P_{k_2}, f_1]_a^b + \cdots + a_{i,2m}[P_{k_2}, f_m]_a^b, \\
&\vdots \\
0 &= [P_{k_m}, G_i]_a^b = 0 + \cdots + 0 + a_{i,m+1}[P_{k_m}, f_1]_a^b + \cdots + a_{i,2m}[P_{k_m}, f_m]_a^b.
\end{aligned}$$

This problem can be recast in terms of the upper half of the finite $2m \times 2m$ matrix \mathbf{M} as above. The upper-left quadrant of \mathbf{M} is then 0. Explicitly, this problem represents the upper-right quadrant of \mathbf{M} multiplied by a column vector of $a_{i,j}$'s. However, the collection $\{P_{k_1}, \dots, P_{k_m}, f_1, \dots, f_m\}$ constitutes a basis for $\mathcal{D}_+ \dot{+} \mathcal{D}_-$, see the remark after the proof of Proposition 3.2.2. Hence, the upper-right quadrant of \mathbf{M} has full rank. The only way to yield the necessary column vectors of 0's, in the above equations, is for all of the $a_{i,j}$'s to be 0. Hence, $a_{i,j} = 0$ for all $j > m$. The calculation was for a general fixed i so necessarily

$$G_i = a_{i,1}P_{k_1} + a_{i,2}P_{k_2} + \cdots + a_{i,m}P_{k_m} \text{ for all } i = 1, \dots, m.$$

The G_i 's themselves must also be linearly independent modulo the minimal domain. So, modulo \mathcal{D}_{\min} , their span is identical to that of $\{P_{k_1}, \dots, P_{k_m}\}$. \square

3.2 GKN Conditions for Powers of the Legendre Operator

When considering a specific differential operator, the problem of finding GKN conditions can be written rather explicitly in terms of the matrix \mathbf{M} from the previous section.

The explicit tools developed here can be adapted to study spectral theory for powers of other Bochner–Krall polynomial systems. Here we focus our attention on the powers of the Legendre operator.

On the one hand, these examples expand the observations in [51]. On the other hand, they motivate and tie into our main results, see Section 3.3. The method established here is more explicit than the abstract approach in Section 3.3.

The investigation into the boundary conditions associated with left-definite theory begins by considering the classical Legendre differential operator $\mathbf{L} = \{\ell, \mathcal{D}_{\mathbf{L}}\}$ on the Hilbert space $L^2(-1, 1)$, given by

$$\ell[y](x) = -((1 - x^2)y'(x))' \quad (3.2.1)$$

together with the domain

$$\mathcal{D}_{\mathbf{L}} = \{f \in \mathcal{D}_{\max}; (1 - x^2)f'(x) \big|_{-1}^1 = 0\} \quad (3.2.2)$$

with connected boundary conditions. This domain contains the Legendre polynomials $\{P_k\}_{k=0}^{\infty}$ and \mathbf{L} is a self-adjoint operator, see e.g. [52]. Recall that \mathcal{D}_{\max} was provided in Definition 2.4.3. Both $\lim_{x \rightarrow \pm 1} (1 - x^2)f'(x)$ exist by Theorem 2.4.4, and because $-(1 - x^2)f'(x) \big|_{-1}^1 = [f, 1] \big|_{-1}^1$.

Remark. In [52], it was proved that $\mathcal{D}_{\mathbf{L}}$ is equal to the domain induced by left-definite theory. The equality of such domains for \mathbf{L}^n is discussed in Section 3.4.

This operator possesses the Legendre polynomials $P_k(x)$, $k \in \mathbb{N}_0$, as a complete set of eigenfunctions. That is, the polynomial $y(x) = P_k(x)$ is a solution of the eigenvalue equation

$$\ell[y](x) = k(k + 1)y(x), \quad (3.2.3)$$

for each k we have $P_k \in \mathcal{D}_{\mathbf{L}}$ and $\text{span}\{P_k\}_{k=0}^{\infty}$ is dense in $L^2(-1, 1)$.

Left-definite theory allows for the construction of a sequence of Hilbert spaces whose domains are operated on by integer composition powers of \mathbf{L} . It is no hindrance that for odd powers of composition, we encounter fractional left-definite spaces, e.g. when $n = 3$ the operator \mathbf{L}^3 corresponds to $\mathcal{V}_{3/2}$. The case $n = 2$ has been investigated by Littlejohn and Wicks in [51] and [52]. They showed that the left-definite

domain in this case could be defined via the GKN1 Theorem using $w_1 \equiv 1$ and $w_2(x) = x$ in equation (2.4.3). The literature does not provide results for $n \geq 3$.

Since the minimal Legendre operator $\mathbf{L}_{\min} = \{\ell, \mathcal{D}_{\min}\}$ has deficiency indices $(1, 1)$ (as is visible from (3.2.2)), the powers $\mathbf{L}_{\min}^n = \{\ell^n, \mathcal{D}_{\min}^n\}$ of the Legendre operator have deficiency indices (n, n) . In other words, we have $m = n$ here.

In the remainder of this section we present a few results for general n , while focusing on some special cases for more explicit results. We are mostly interested in $n = 3$, but also work with $n = 4$ and $n = 5$, and include some new observations when $n = 2$.

3.2.1 The Structure of the Matrix \mathbf{M}_n

These explicit results can be extended by analogy to larger values of n . For general n , the matrix \mathbf{M}_n will be $(2n) \times (2n)$ and the entries are sesquilinear forms corresponding to expression ℓ^n in Green's formula. If n is even, choose P_0, P_1, \dots, P_{n-1} and Q_0, Q_1, \dots, Q_{n-1} (Legendre functions of the second kind). If n is odd, choose P_0, P_1, \dots, P_{n-1} and Q_1, Q_2, \dots, Q_n . These will be the choice for basis candidates unless otherwise stated. In the following example we explain why these are good choices. Apart from its pedagogical value, this example also settles the case $n = 3$ with little computational effort. The case $n = 2$ was the main topic of [51].

Example. Let $n = 3$. The first two Legendre polynomials are $P_0 \equiv 1$ and $P_1(x) = x$, so a reasonable guess in this case would be to try to use as GKN conditions

$$P_0 \equiv 1, \quad P_1(x) = x, \quad P_2(x) = \frac{1}{2}(3x^2 - 1).$$

It will be shown that these GKN conditions indeed yield the desired domain. The most difficult condition to prove is the linear independence modulo the minimal domain. For $n = 3$, the deficiency indices are $(3, 3)$. So we have $m = n = 3$ and a basis of $\mathcal{D}_+^3 \dot{+} \mathcal{D}_-^3$ will be $2n = 6$ dimensional.

To show that a set w_1, w_2, \dots, w_6 is linearly independent modulo \mathcal{D}_{\min}^3 , follow the setup of the matrix described in Subsection 3.1.3 to yield

$$\mathbf{M}_3 = \left(\begin{array}{ccc|ccc} [w_1, w_1] & [w_1, w_2] & [w_1, w_3] & [w_1, w_4] & [w_1, w_5] & [w_1, w_6] \\ [w_2, w_1] & [w_2, w_2] & [w_2, w_3] & [w_2, w_4] & [w_2, w_5] & [w_2, w_6] \\ [w_3, w_1] & [w_3, w_2] & [w_3, w_3] & [w_3, w_4] & [w_3, w_5] & [w_3, w_6] \\ \hline [w_4, w_1] & [w_4, w_2] & [w_4, w_3] & [w_4, w_4] & [w_4, w_5] & [w_4, w_6] \\ [w_5, w_1] & [w_5, w_2] & [w_5, w_3] & [w_5, w_4] & [w_5, w_5] & [w_5, w_6] \\ [w_6, w_1] & [w_6, w_2] & [w_6, w_3] & [w_6, w_4] & [w_6, w_5] & [w_6, w_6] \end{array} \right),$$

where $[\cdot, \cdot]$ stands for the sesquilinear form in equation (3.4.1) below for $n = 3$ and is evaluated from -1 to 1 by taking limits.

For one moment, let us assume that all those limits exist. Now the idea is that we will be choosing all of the w_j to be either Legendre eigenfunctions or Legendre functions of the second kind, all of which satisfy eigenvalue equations $\ell[y] = \lambda y$. The representation through Green's formula

$$[w_j, w_k] \Big|_{-1}^1 = \int_{-1}^1 \ell^3[w_j] w_k dx - \int_{-1}^1 w_j \ell^3[w_k] dx$$

will be of use.

The Legendre functions of the second kind are commonly denoted by Q_k , $k \in \mathbb{N}_0$. The explicit representations for the first four of them are:

$$\begin{aligned} Q_0(x) &= \frac{1}{2} \ln \left(\frac{1+x}{1-x} \right), & Q_1(x) &= \frac{x}{2} \ln \left(\frac{1+x}{1-x} \right) - 1, \\ Q_2(x) &= \frac{3x^2 - 1}{4} \ln \left(\frac{1+x}{1-x} \right) - \frac{3x}{2}, & Q_3(x) &= \frac{5x^3 - 3x}{4} \ln \left(\frac{1+x}{1-x} \right) - \frac{5x^2}{2} + \frac{2}{3}. \end{aligned}$$

More information about these functions can be found in [20, 59]. Explicitly, take

$$w_1 = P_0, \quad w_2 = P_1, \quad w_3 = P_2, \quad \text{and} \quad w_4 = Q_1, \quad w_5 = Q_2, \quad w_6 = Q_3.$$

Let us ensure that the limits in these sesquilinear forms are well-defined. ✦

We turn back to general n . Since P_k are eigenfunctions, they trivially belong to \mathcal{D}_{\max}^n . In conjunction with Theorem 2.4.4 the following result shows that the limits of the sesquilinear forms $\lim_{x \rightarrow -1+} [w_j, w_k](x)$ and $\lim_{x \rightarrow 1-} [w_j, w_k](x)$ both exist when w_j and w_k are eigenfunctions or polynomials of the second kind.

Proposition 3.2.1. *The Legendre functions of the second kind are in the maximal domain \mathcal{D}_{\max}^n for every value of n .*

Proof. By Definition 2.4.3 the maximal domain of ℓ^n is given by

$$\mathcal{D}_{\max}^n = \left\{ y : (-1, 1) \rightarrow \mathbb{C} \mid y^{(k)} \in \text{AC}_{\text{loc}}(-1, 1), \quad k=0, 1, \dots, 2n-1; \right. \\ \left. y, \ell^n[y] \in L^2(-1, 1) \right\}.$$

These functions are in $L^2(-1, 1)$ and their integrals are explicitly known [20]:

$$\int_{-1}^1 (Q_k(x))^2 dx = \frac{\pi^2 - 2(1 + \cos^2(k\pi))\psi'(k+1)}{2(2k+1)},$$

where the function $\psi(x) = \Gamma'(x)/\Gamma(x)$ is the so-called digamma function. Derivatives of the functions Q_k have singularities only at -1 and 1 , so $Q_k^{(r)} \in C^\infty[\alpha, \beta]$ for all $r \in \mathbb{N}$ and all $[\alpha, \beta] \subset (-1, 1)$. Hence, each derivative is itself locally continuously differentiable and locally absolutely continuous. The fact that the functions Q_k are solutions to the eigenvalue equation (3.2.3) trivially implies that $\ell^n[Q_k] \in L^2(-1, 1)$ for all $k \in \mathbb{N}_0$. \square

Initial conclusions can be made about the structure of \mathbf{M}_n using technical facts about the entries. In the remainder of this section we will always assume that the first n of the w_j are Legendre polynomials and the others are Legendre functions of the second kind (with indices in \mathbb{N}_0).

Proposition 3.2.2. *The matrix \mathbf{M}_n is antisymmetric and takes the form*

$$\mathbf{M}_n = \left(\begin{array}{c|c} \mathbf{0} & \mathbf{B}_n \\ \hline -\mathbf{B}_n^\top & \mathbf{C}_n \end{array} \right)$$

so that $\det(\mathbf{M}_n) = \det(\mathbf{B}_n^\top \mathbf{B}_n) = [\det(\mathbf{B}_n)]^2$. In particular, if \mathbf{B}_n has full rank, then the w_j used to produce the entries of \mathbf{M}_n form a basis of \mathcal{D}_{\max} modulo \mathcal{D}_{\min} .

Proof. Simplify the entries of the matrix \mathbf{M} by using Green's formula (2.4.1) as follows: For $f_j = P_j$ or $f_j = Q_j$ and $g_k = P_k$ or $g_k = Q_k$ and with the standard inner product $\langle \cdot, \cdot \rangle$ on $L^2(-1, 1)$, notice that

$$\begin{aligned} [f_j, g_k] \Big|_{-1}^1 &= \langle \ell^n[f_j], g_k \rangle - \langle f_j, \ell^n[g_k] \rangle = [j^n(j+1)^n - k^n(k+1)^n] \langle f_j, g_k \rangle \quad (3.2.4) \\ &= -[k^n(k+1)^n - j^n(j+1)^n] \langle f_j, g_k \rangle = \langle f_j, \ell^n[g_k] \rangle - \langle \ell^n[f_j], g_k \rangle \\ &= -[g_k, f_j] \Big|_{-1}^1. \end{aligned}$$

Here, we used that repeated applications of the eigenvalue equation (3.2.3) yield $\ell^n[P_k] = k^n(k+1)^n P_k$, and similarly for Q_k . This shows antisymmetry.

In the first quadrant of the matrix, we encounter the case when the sesquilinear form is evaluated for two Legendre polynomials. Due to the orthogonality of the inner product, (3.2.4) evaluates to zero when $f_j = P_j$ and $g_k = P_k$ when $j \neq k$. For $j = k$, the coefficient in front of the inner product equals zero. Summing up, this shows

$$[P_j, P_k] \Big|_{-1}^1 = 0, \text{ for all } j, k \in \mathbb{N}_0.$$

By linear algebra, the determinant of \mathbf{M} can be calculated using

$$\det(\mathbf{M}_n) = \det[(\mathbf{0}^\top)(\mathbf{C}_n) - (-\mathbf{B}_n^\top)(\mathbf{B}_n)] = \det(\mathbf{B}_n^\top \mathbf{B}_n) = [\det(\mathbf{B}_n)]^2.$$

The last statement follows from Corollary 3.1.8. □

Remark. In fact, it is not difficult to see that this proof works in more general settings. Namely, \mathbf{M}_n has the structure of Proposition 3.2.2 any time we choose eigenfunctions for w_1 through w_n .

Several immediate consequences of equation (3.2.4) regarding the particular entries of \mathbf{M}_n are now apparent. As before, let $f_j = P_j$ or $f_j = Q_j$ and $g_k = P_k$ or

$g_k = Q_k$. First notice that

$$[f_j, g_k] \Big|_{-1}^1 = 0 \quad \text{for } j = k.$$

Fortunately, formulas are known to calculate the relevant inner products [59, pp. 236], and also exist in the cases where two different P_j 's and two different Q_k 's are considered: When both functions are Legendre functions of the second kind it is known that

$$\langle Q_j, Q_k \rangle = \frac{[\psi(j+1) - \psi(k+1)][1 + \cos(j\pi) \cos(k\pi)] + \frac{1}{2}\pi \sin((k-j)\pi)}{(k-j)(j+k+1)} \quad \text{for } j \neq k.$$

The case where the functions are of mixed type is given by

$$\langle P_j, Q_k \rangle = \frac{2 \sin(j\pi) \cos(k\pi) [\psi(j+1) - \psi(k+1)] + \pi \cos((k-j)\pi) - \pi}{\pi(k-j)(j+k+1)} \quad \text{for } j \neq k.$$

The function $\psi(x)$ is the digamma function in the above two formulas.

The formulas are only necessary for $j, k \in \mathbb{N}_0$, reducing the computations significantly. In particular, for $j, k \in \mathbb{N}_0$:

$$\begin{aligned} [Q_j, Q_k] \Big|_{-1}^1 & \quad (3.2.5) \\ = \begin{cases} \frac{2[\psi(j+1) - \psi(k+1)][j^3(j+1)^3 - k^3(k+1)^3]}{(k-j)(j+k+1)} =: \Phi_{jk}, & j+k \text{ even and } j \neq k, \\ 0, & j+k \text{ odd or } j = k. \end{cases} \end{aligned}$$

Analogously, for $j, k \in \mathbb{N}_0$:

$$[P_j, Q_k] \Big|_{-1}^1 = \begin{cases} \frac{-2[j^3(j+1)^3 - k^3(k+1)^3]}{(k-j)(j+k+1)} =: \varphi_{jk}, & j+k \text{ odd}, \\ 0, & j+k \text{ even}. \end{cases} \quad (3.2.6)$$

The definition of the matrix entries given in equations (3.2.5) and (3.2.6) immediately yield that $\Phi_{jk} = -\Phi_{kj}$ and $\varphi_{jk} = -\varphi_{kj}$. In particular, the blocks \mathbf{B}_n and

\mathbf{C}_n from Proposition 3.2.2 can be explicitly computed for even n as

$$\mathbf{B}_n = \begin{pmatrix} 0 & \varphi_{01} & 0 & \varphi_{03} & \dots & \varphi_{0(n-1)} \\ \varphi_{10} & 0 & \varphi_{12} & 0 & \dots & 0 \\ 0 & \varphi_{21} & 0 & \varphi_{23} & \dots & \varphi_{2(n-1)} \\ \varphi_{30} & 0 & \varphi_{32} & 0 & \dots & 0 \\ 0 & \varphi_{41} & 0 & \varphi_{43} & \dots & \varphi_{4(n-1)} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \varphi_{(n-1)0} & 0 & \varphi_{(n-1)2} & 0 & \dots & 0 \end{pmatrix},$$

$$\mathbf{C}_n = \begin{pmatrix} 0 & 0 & \Phi_{02} & 0 & \dots & 0 \\ 0 & 0 & 0 & \Phi_{13} & \dots & \Phi_{1(n-1)} \\ \Phi_{20} & 0 & 0 & 0 & \dots & 0 \\ 0 & \Phi_{31} & 0 & 0 & \dots & \Phi_{3(n-1)} \\ \Phi_{40} & 0 & \Phi_{42} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \Phi_{(n-1)1} & 0 & \Phi_{(n-1)3} & \dots & 0 \end{pmatrix}.$$

The case where n is odd can similarly be written down in terms of the above formulas.

Mathematica can be used to ease the trouble of populating the matrix with the relevant entries.

Example. We return to the case $n = 3$. The following matrix is the result of setting $w_1 = P_0$, $w_2 = P_1$, $w_3 = P_2$, $w_4 = Q_1$, $w_5 = Q_2$, and $w_6 = Q_3$:

$$\mathbf{M}_3 = \left(\begin{array}{ccc|ccc} & & & 8 & 0 & 288 \\ & & & 0 & 104 & 0 \\ & & & 104 & 0 & 504 \\ \hline & & & \hline -8 & 0 & -104 & 0 & 0 & \frac{860}{3} \\ 0 & -104 & 0 & 0 & 0 & 0 \\ -288 & 0 & -504 & \frac{-860}{3} & 0 & 0 \end{array} \right).$$

Now, the upper right quadrant \mathbf{B}_3 of \mathbf{M}_3 clearly has full rank. And, in accordance with Proposition 3.2.2, we obtain that w_1, \dots, w_6 form a basis of \mathcal{D}_{\max} modulo \mathcal{D}_{\min} .

Now, Corollary 3.1.8 asserts that these are in fact the desired GKN conditions for the cube of the Legendre differential operator. \star

In virtue of Proposition 3.2.2 higher values of n are more easily accessible, as they are less computationally expensive and the digamma function in the lower right quadrant is avoided.

The cases where $n = 4$ and $n = 5$ are included below to illustrate how this method can be generalized.

Example. For $n = 4$ choose the functions P_0, \dots, P_3 and Q_0, \dots, Q_3 as candidates for basis vectors. The relevant matrix can be computed to be:

$$\mathbf{B}_4 = \begin{pmatrix} 0 & 16 & 0 & 3456 \\ 16 & 0 & 640 & 0 \\ 0 & 640 & 0 & 6480 \\ 3456 & 0 & 6480 & 0 \end{pmatrix}.$$

This matrix is of particular interest, because it is representative of all cases where n is even and the basis vectors are chosen to be P_0, \dots, P_{n-1} and Q_0, \dots, Q_{n-1} . In these cases, the matrix \mathbf{B}_n is symmetric.

The invertibility of \mathbf{B}_4 immediately reduces to showing that both submatrices

$$\begin{pmatrix} 16 & 3456 \\ 640 & 6480 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 16 & 640 \\ 3456 & 6480 \end{pmatrix}$$

have non-zero determinant. This is trivially true.

Therefore, the GKN conditions P_0, \dots, P_3 yield a self-adjoint operator and since all eigenfunctions P_k satisfy these conditions, we obtain the left-definite operator that is associated with \mathbf{L}^4 . ✱

Example. For $n = 5$ choose the functions P_0, \dots, P_4 and Q_1, \dots, Q_5 as candidates for basis vectors. The relevant matrix can be computed to be:

$$\mathbf{B}_5 = \begin{pmatrix} 32 & 0 & 41472 & 0 & 1620000 \\ 0 & 3872 & 0 & 355552 & 0 \\ 3872 & 0 & 80352 & 0 & 2024352 \\ 0 & 80352 & 0 & 737792 & 0 \\ 355552 & 0 & 737792 & 0 & 4220000 \end{pmatrix}.$$

Again, it can easily be shown that \mathbf{B}_5 has full rank. ✱

Example. Matlab has allowed us to verify that the first n Legendre polynomials are suitable for \mathbf{L}^n when $n \leq 16$. Vast stratification in magnitude of matrix entries is responsible for this *early* failing of the numerical computations. ✱

3.2.2 Necessary Condition and Conjecture

It is clear the methods developed above are powerful, albeit limited to calculation, and can be expressed in more generality. Apart from increasing n , another way to generalize stems from choosing a more general set of indices for the Legendre polynomials, and for the Legendre functions of the second kind, as hinted at in Theorem 3.1.6.

There is a necessary condition for the truncated matrix \mathbf{B}_n having full rank which requires some additional requirements on the indices of both the Legendre polynomials and the Legendre functions of the second kind.

Proposition 3.2.3. Let \mathbf{M}_n define a basis of functions for the space $\mathcal{D}_+^n + \mathcal{D}_-^n$ when n is general. Let the choice of functions for this basis be $P_{j_1}, P_{j_2}, \dots, P_{j_n}$ and $Q_{k_1}, Q_{k_2}, \dots, Q_{k_n}$. Define $\mathfrak{J} := \{j_1, \dots, j_n, k_1, \dots, k_n\}$ be the collection of indices for these functions. Then \mathfrak{J} contains n even and n odd elements.

Proof. Assume \mathbf{M}_n has full rank, so that $P_{j_1}, P_{j_2}, \dots, P_{j_n}$ and $Q_{k_1}, Q_{k_2}, \dots, Q_{k_n}$ are indeed a basis for \mathcal{D}_{\max} modulo \mathcal{D}_{\min} . Without loss of generality, also assume that there are more even numbers in \mathfrak{J} than odd numbers. By Proposition 3.2.2, the Glazman conditions and anti-symmetry of the matrix then completely reduces our problem to showing that \mathbf{B}_n does not have full rank.

Recall that the (i, l) -entry of \mathbf{B}_n equals $[P_{j_i}, Q_{k_l}]|_{-1}^1$ for $1 \leq i, l \leq n$ and is given by equation (3.2.6). So, these entries are only nonzero when $j_i + k_l$ is odd. Hence, interchange rows of \mathbf{B}_n to group the even indices first for the set of P_{j_i} 's, and interchange columns to group the even indices first for the set of Q_{k_l} 's. This creates two blocks of entries on the anti-diagonal in the upper right quadrant, where the P index is even and the Q index is odd, and one where the P index is odd and the Q index is even. The rank of \mathbf{B}_n is the sum of the rank of these two blocks. However, because there are more even indices than odd ones, neither of these blocks are square, so the sum of their ranks cannot be equal to n . This means \mathbf{M}_n cannot have rank $2n$, which is a contradiction. Therefore, the number of even and odd numbers in the set \mathfrak{J} must be equal. \square

The matrix \mathbf{B}_n raises several important questions concerning the rules that are necessary and/or sufficient on the indices (other than the requirement of Proposition 3.2.3 above) in order to ensure that the \mathbf{B}_n has rank n . Unfortunately, the answer

to this question can only be conjectured currently. Progress in this direction using theoretical aspects of the setup is shown in the next two sections.

Conjecture 3.2.4. Let $P_{j_1}, P_{j_2}, \dots, P_{j_n}$ be any set of n distinct Legendre polynomials, with n_1 odd indices and n_2 even indices so that $n_1 + n_2 = n$. Then these Legendre polynomials can be used as GKN conditions to define the $n/2$ left-definite domain.

In particular, choose any n distinct Legendre functions of the second kind $Q_{k_1}, Q_{k_2}, \dots, Q_{k_n}$ with n_2 odd indices and n_1 even indices. Then together these $2n$ functions constitute a basis of the space $\mathcal{D}_+^n \dot{+} \mathcal{D}_-^n$.

Immediate inspiration for the conjecture stems from the $n = 2$ case.

Example. Consider the $n = 2$ case for simplicity. If one odd index and one even index are chosen for the P_j 's (say P_j and P_k with even j and odd k) then the claim follows: \mathbf{B}_2 only has entries on the anti-diagonal and hence is rank 2. \clubsuit

Example. Now, again for $n = 2$, assume that both chosen indices are odd, so that both of the indices for the Q_k 's are even. As a further simplification, choose Q_0 and Q_2 . The matrix of interest is

$$\mathbf{B}_2 = \begin{pmatrix} \varphi_{j0} & \varphi_{j2} \\ \varphi_{k0} & \varphi_{k2} \end{pmatrix},$$

where j and k are both odd.

To reduce to row echelon form, the row operation necessary is $\alpha\varphi_{j0} + \varphi_{k0} = 0$ so that $\alpha = -\varphi_{k0}/\varphi_{j0}$. This changes φ_{k2} to be $\tilde{\varphi}_{k2} = \alpha\varphi_{j2} + \varphi_{k2}$. This can be written out explicitly to be

$$\begin{aligned} \tilde{\varphi}_{k2} = & ((k^2(k+1)^2) - 1)(j^2(j+1)^2 - 36)(j^2 + j)(-k^2 - k + 6) \\ & - ((j^2(j+1)^2) - 1)(k^2(k+1)^2 - 36)(k^2 + k)(-j^2 - j + 6). \end{aligned}$$

Mathematica shows that $\tilde{\varphi}_{k2} = 0$ has no solutions for distinct j and k , where both are odd and positive. A similar equation is relevant for the case where both j and k are

even and Q_1 and Q_3 are chosen as the paired basis vectors. Mathematica similarly shows it is not possible to get j and k to be distinct, even and positive. This shows that any 2 distinct indices for the Legendre polynomials will be sufficient to define the first left-definite domain via GKN conditions. \clubsuit

There is further evidence that the conjecture is true.

Example. Let $n = 4$ and choose the functions $P_{17}, P_{42}, P_{49}, P_{125}$ and $Q_{24}, Q_{82}, Q_{97}, Q_{178}$ as candidates for the basis vectors. The relevant matrix can be computed to be:

$$\mathbf{B}_4 = \begin{pmatrix} 821988432 & 660210828928 & 0 & 65319097828480 \\ 0 & 0 & 2118187203328 & 0 \\ 38811250000 & 968624405632 & 0 & 70078111267456 \\ 8123415750000 & 13280257143232 & 0 & 120291674577856 \end{pmatrix}.$$

It is not hard to see that this matrix possesses full rank. \clubsuit

Unfortunately, the complexity of the matrix operations and higher values for n mean verifying that solutions are not of the desired form is computationally expensive. However, to add a little more weight to the conjecture, the above form can be easily adapted to the $n = 3, 4$ cases where there are two even or two odd choices of indices of the P_j 's. In conclusion the assertion in the conjecture about the choice of indices for the P_j 's is verified using Mathematica for $n = 2$, and it is true in special cases when $n = 3$ and $n = 4$.

3.3 Eigenfunctions in General Left-Definite Theory

The following theorems apply to general left-definite settings so it is imperative to clarify some of the subtler points of abstraction. It should be understood that the differential expression that is being generated from left-definite theory is not changing under the classical extension theory, only that the minimal domain is being augmented to include more functions and become self-adjoint. Specifically, \mathbf{L}_{\min} and \mathbf{L} possess domains \mathcal{D}_{\min} and $\mathcal{D}_{\mathbf{L}}$ respectively, but both operate on functions using $\ell[\cdot]$. Also,

recall that an operator defined by left-definite theory means that it is generated by composing self-adjoint differential operators with themselves to create a Hilbert scale of operators. The domains of these operators shrink as the number of compositions increase. For more details refer to Section 2.3.

The following results play the role of an indicator for identifying left-definite domains in terms of GKN conditions.

Theorem 3.3.1. Let \mathbf{L} be a self-adjoint operator defined by left-definite theory on $L^2[(a, b), w]$ with domain $\mathcal{D}_{\mathbf{L}}$ (which is a restriction of the maximal domain \mathcal{D}_{\max}) that includes a complete orthogonal system of eigenfunctions. Enumerate the eigenfunctions as $\{P_k\}_{k=0}^{\infty}$. Furthermore, let \mathbf{L} be an extension of the minimal (symmetric, closed) operator \mathbf{L}_{\min} with domain \mathcal{D}_{\min} , where \mathbf{L} and \mathbf{L}_{\min} operate on their respective domains by $\ell[\cdot]$, and \mathbf{L}_{\min} has deficiency indices (m, m) .

Then, the GKN conditions for the self-adjoint operator \mathbf{L} are given by some $\{P_{k_1}, \dots, P_{k_m}\}$.

Remark. It was pointed out to us by one of the reviewers that this result probably does not critically hinge on the left-definite setting. We expect the conclusions to be true for any self-adjoint operator with a complete system of eigenfunctions.

Proof. The case $m = 0$ is trivial, since then $\mathbf{L}_{\min} = \mathbf{L} = \mathbf{L}_{\max}$. Let $m \geq 1$.

The main work lies in showing that some of the eigenfunctions yield appropriate choices for w_1, \dots, w_m from the perspective of Theorem 2.4.9 (the GKN1 Theorem). That is, we need to show that there are m members $\{P_{k_1}, \dots, P_{k_m}\}$ of the collection $\{P_k\}_{k=0}^{\infty}$, which both satisfy the Glazman symmetry conditions (2.4.4) and are linearly independent modulo the minimal domain \mathcal{D}_{\min} , see Definition 2.4.8.

First, we show that all possible choices of $\{P_{k_1}, \dots, P_{k_m}\}$ satisfy the Glazman symmetry conditions. Recall that an application of the Green's formula for the sesquilinear form yields $[P_i, P_j]_a^b = 0$ for $i, j \in \mathbb{N}_0$, see equation (3.1.4).

Next, we show that there exist functions $\{P_{k_1}, \dots, P_{k_m}\}$ that are linearly independent modulo \mathcal{D}_{\min} . Part (2) of Lemma 3.1.3 states that the maximal domain decomposes orthogonally with respect to graph norm into $\mathcal{D}_{\max} = \mathcal{D}_{\min} \oplus_{\mathbf{A}} \mathcal{D}_+ \oplus_{\mathbf{A}} \mathcal{D}_-$. Define the auxiliary functions $\{\tilde{P}_k\}_{k=0}^\infty$ to be the orthogonal projection (in accordance with the graph norm) of the P_k 's onto $\mathcal{D}_+ \oplus_{\mathbf{A}} \mathcal{D}_-$.

Recall that \mathbf{L}_{\min} has defect indices (m, m) and that the subspaces satisfy

$$\mathcal{D}_{\min} < \mathcal{D}_{\mathbf{L}} < \mathcal{D}_{\max}.$$

Since \mathbf{L} is self-adjoint, we have that $\mathcal{D}_{\mathbf{L}} \ominus_{\mathbf{A}} \mathcal{D}_{\min}$ is m dimensional. The projection is orthogonal, so $\{\tilde{P}_k\}_{k=0}^\infty$ spans an m dimensional subspace of $\mathcal{D}_+ \oplus_{\mathbf{A}} \mathcal{D}_-$, the closure being taken with respect to the graph norm. Indeed, assume this dimension was strictly less than m . The orthogonality of the projection also means that our assumption would imply that the closure in graph norm of $\text{span}\{P_k\}_{k=0}^\infty$ is a proper subspace of $\mathcal{D}_{\mathbf{L}}$. Lemma 3.1.4 says the graph norm and the norm in the corresponding left-definite space are equivalent. However, Theorem 2.3.4 states that $\mathcal{D}_{\mathbf{L}}$ is equal to the closure in the norm induced in the second left-definite space associated with the pair $(\mathcal{H}, \mathbf{A}) = (L^2[(a, b), w], \mathbf{L})$. This is a contradiction, so the $\{\tilde{P}_k\}_{k=0}^\infty$ span an m dimensional subspace of $\mathcal{D}_+ \oplus_{\mathbf{A}} \mathcal{D}_-$.

This means that the problem is now finite dimensional! In particular, the closure of spans is obvious. Also, there are m functions $\{\tilde{P}_{k_i}\}_{i=1}^m$ which can be completed to a basis $\{\tilde{P}_{k_1}, \dots, \tilde{P}_{k_m}, h_1, \dots, h_m\}$ of $\mathcal{D}_+ \oplus_{\mathbf{A}} \mathcal{D}_-$. Therefore, the functions $\{\tilde{P}_{k_i}\}_{i=1}^m$ are linear independent modulo \mathcal{D}_{\min} .

The definition of \tilde{P}_k implies $P_k - \tilde{P}_k \in \mathcal{D}_{\min}$. Hence, when viewed in the quotient space $\mathcal{D}_{\max} \ominus \mathcal{D}_{\min}$, the projection \tilde{P}_k belongs to the same equivalence class as the corresponding eigenfunction P_k , $[\tilde{P}_k] = [P_k]$. Invoking the definition of linear independence modulo \mathcal{D}_{\min} again, the eigenfunctions $\{P_{k_i}\}_{i=1}^m$ are linearly independent modulo the minimal domain.

Therefore, there are m members of $\{P_{k_i}\}_{i=1}^m$ which define a self-adjoint extension $\tilde{\mathbf{L}}$ of \mathbf{L}_{\min} in the above fashion, via the GKN1 Theorem (Theorem 2.4.9). It remains to verify that $\tilde{\mathbf{L}} = \mathbf{L}$. From equation (3.1.4) we immediately conclude that all of the $\{P_k\}_{k=0}^\infty$ belong to the domain $\mathcal{D}_{\tilde{\mathbf{L}}}$. Thus $\mathbf{L} \subseteq \tilde{\mathbf{L}} \subseteq \tilde{\mathbf{L}}^* \subseteq \mathbf{L}^*$, and it is known that $\mathbf{L} = \mathbf{L}^*$. \square

This theorem relied heavily on the GKN1 Theorem and began with a self-adjoint operator generated by left-definite theory to define the boundary conditions imposed to create the left-definite space. However, the GKN theory goes both ways to create a complete framework of both necessary and sufficient conditions. The similar conditions of the GKN2 Theorem allow another statement to be made.

Corollary 3.3.2. Let \mathbf{L} be as in Theorem 3.3.1. Then the $2n$ th (for $n \in \mathbb{N}$) left-definite space generated by the operator \mathbf{L} will have deficiency indices (nm, nm) . Further, the GKN conditions for the $2n$ th left-definite space are given by some $\{P_{k_1}, \dots, P_{k_{nm}}\}$.

Proof. The $2n$ th left-definite space exists and is unique for the operator \mathbf{L} . It also possesses the complete set of orthogonal eigenfunctions that are in the domain of \mathbf{L} , and their spectra coincide. Glazman symmetry conditions and the linear independence of $\{P_{k_1}, \dots, P_{k_{nm}}\}$ modulo the minimal domain follow by the same argument as the previous theorem. Indices matching the $2n$ th left-definite space with the n th power composition of the operator follows from Corollary 2.3.3. The result follows by the GKN2 Theorem. \square

This corollary provides a complete answer to the question of which functions should be considered as GKN conditions to create left-definite spaces. The only further improvement would be to explicitly say which eigenfunctions were sufficient for this purpose. The next section seeks to answer this question when the operator stems from a Sturm–Liouville differential expression.

3.4 Left-Definite Domains of Sturm–Liouville Operators

Let \mathbf{L}^n be a self-adjoint operator defined by left-definite theory on $L^2[(a, b), w]$ with domain $\mathcal{D}_{\mathbf{L}}^n$ that includes a complete system of orthogonal eigenfunctions. Let \mathbf{L}^n operate on its domain via $\ell^n[\cdot]$, a differential operator of order $2n$, where $n \in \mathbb{N}$, generated by composing a Sturm–Liouville differential operator with itself n times. Furthermore, let \mathbf{L}^n be an extension of the minimal operator \mathbf{L}_{\min}^n , which has deficiency indices (m, m) .

As we are working with coupled boundary conditions for the n th power of an operator, it suffices to consider $m = n$. Let us explain why. The case where $m = n$ corresponds to both endpoints of ℓ being limit circle. If only one endpoint is limit point, then one GKN condition is still necessary for ℓ . This GKN condition then imposes a restriction at the limit circle endpoint, while it is just satisfied trivially on the limit point side by all functions in the maximal domain. If both endpoints are limit point, then no boundary conditions are needed. In that case \mathbf{L}_{\min} is essentially self-adjoint. Therefore, we assume without loss of generality that the deficiency indices are (n, n) in this section. A more in depth discussion can be found in [9, 54, 65–67] and Subsection 2.2.1.

Enumerate the orthogonal eigenfunctions as $\{P_k\}_{k=0}^\infty$. Define the following domains:

$$\begin{aligned}\mathcal{A}_n &:= \left\{ f \in \mathcal{D}_{\max}^n \mid f, f', \dots, f^{(2n-1)} \in AC_{\text{loc}}(a, b); (p(x))^n f^{(2n)} \in L^2[(a, b), w] \right\}, \\ \mathcal{B}_n &:= \left\{ f \in \mathcal{D}_{\max}^n \mid [f, P_j]_n \Big|_a^b = 0 \text{ for } j = 0, 1, \dots, n-1 \right\}, \\ \mathcal{C}_n &:= \left\{ f \in \mathcal{D}_{\max}^n \mid [f, P_j]_n \Big|_a^b = 0 \text{ for some } n \text{ distinct } j \in \mathbb{N} \right\}, \text{ and} \\ \mathcal{F}_n &:= \left\{ f \in \mathcal{D}_{\max}^n \mid (a_j(x) f^{(j)}(x))^{(j-1)} \Big|_a^b = 0 \text{ for } j = 1, 2, \dots, n \right\}.\end{aligned}$$

The $p(x)$ above is from the standard definition of a Sturm–Liouville differential operator, given in equation (2.2.2), and the $a_j(x)$ ’s are from the Lagrangian symmetric form of the operator in (2.2.3). These domains seem very different, yet progress has

already been made in this paper and elsewhere on the equality of these domains. The n th left-definite domain, $\mathcal{D}_{\mathbf{L}}^n$ is found to be equal to \mathcal{A}_n for the Legendre differential operator in [52, Section 7.5]. A general form for $\mathcal{D}_{\mathbf{L}}^n$ is missing from the literature, so we will assume it is equal to \mathcal{A}_n for the rest of this section. Indeed, the main condition of \mathcal{A}_n simply involves the term associated with $f^{(2n)}$ when $\ell^n[f]$ is decomposed into a sum of derivatives of f . There is a proof of $\mathcal{A}_n \subseteq \mathcal{F}_n$ in [52] for the special case where the differential operator $\ell^n[\cdot]$ denotes the n^{th} composite power of the Legendre differential expression and the eigenfunctions $\{P_k\}_{k=0}^{\infty}$ are the Legendre polynomials. This scenario for small n was discussed in Section 3.2. The conditions in \mathcal{F}_n are particularly significant as they represent easily testable conditions that are not in the GKN format.

In Section 3.3 it was shown that by a proper re-enumeration of the eigenfunctions $\{P_k\}_{k=0}^{\infty}$, we have $\mathcal{A}_n = \mathcal{B}_n$. There we also proved $\mathcal{A}_n = \mathcal{B}_n = \mathcal{C}_n$ for $n=2$ in the Legendre setting (see the first example after Conjecture 3.2.4). However, a proof of the general n case for $\mathcal{A}_n = \mathcal{B}_n = \mathcal{C}_n$ is elusive at this stage. It is obvious that $\mathcal{B}_n \subset \mathcal{C}_n$.

Conjecture 3.4.1. Let \mathbf{L}^n be a self-adjoint operator defined by left-definite theory on $L^2[(a, b), w]$ with domain $\mathcal{D}_{\mathbf{L}}^n$ that includes a complete system of orthogonal polynomial eigenfunctions, that is, we use $\mathcal{D}_{\mathbf{L}}^n = \mathcal{A}_n$. Let \mathbf{L}^n operate on its domain via $\ell^n[\cdot]$, a differential operator of order $2n$, where $n \in \mathbb{N}$, generated by composing a Sturm–Liouville differential operator with itself n times. Furthermore, let \mathbf{L}^n be an extension of the minimal operator \mathbf{L}_{\min}^n , which has deficiency indices (n, n) . Then $\mathcal{A}_n = \mathcal{B}_n = \mathcal{C}_n = \mathcal{F}_n = \mathcal{D}_{\mathbf{L}}^n \forall n \in \mathbb{N}$.

This conjecture extends one made in [52, Chapter 9] by the broad conditions in \mathcal{C}_n . Here we prove some subcases.

Theorem 3.4.2. *Under the hypotheses of Conjecture 3.4.1, and the assumption that $\mathcal{A}_n = \mathcal{B}_n$, we have $\mathcal{B}_n \subseteq \mathcal{F}_n \forall n \in \mathbb{N}$.*

The proof utilizes an explicit form of the sesquilinear form, as opposed to the one given in equation (2.4.1). This representation allows for more precision in defining which limits are disappearing and which are remaining as we approach the endpoints of (a, b) . For many of the Sturm–Liouville operators of interest the expression $q(x)/w(x)$ is a constant, and we have

$$[f, g]_n(x) = \sum_{k=1}^n \sum_{j=1}^k (-1)^{k+j} \left\{ (a_k(x) \bar{g}^{(k)}(x))^{(k-j)} f^{(j-1)}(x) \right. \\ \left. - (a_k(x) f^{(k)}(x))^{(k-j)} \bar{g}^{(j-1)}(x) \right\}, \quad (3.4.1)$$

where the $a_k(x)$'s are again from the Lagrangian symmetric form of the differential operator (2.2.3). For a reference in the Legendre setting, see e.g. [51, Section 10]. One of the reviewers pointed out to us that many other examples such as Exceptional Orthogonal Polynomials will also satisfy the hypotheses of Conjecture 3.4.1 and Theorem 3.4.2.

Proof of Theorem 3.4.2. We proceed by induction on n . The base case is proven by a simple application of Green's Formula for the sesquilinear form. Let $f \in \mathcal{B}_1$. We compute

$$0 = [f, P_0]_1|_a^b = [f, 1]_1|_a^b = \langle \ell[f], 1 \rangle_{L^2[(a,b),w]} - \langle f, \ell[1] \rangle_{L^2[(a,b),w]} \\ = \int_a^b \left(\frac{1}{w(x)} [p(x)f'(x)]' \right) w(x) dx - 0 = \lim_{x \rightarrow b^-} (p(x)f'(x)) - \lim_{x \rightarrow a^+} (p(x)f'(x)),$$

where the term involving q cancels out (as it is added and then subtracted).

Assume that $\mathcal{B}_{n-1} \subseteq \mathcal{F}_{n-1}$ as the inductive hypothesis. Corollary 2.3.3 shows that

$$\mathcal{D}_{\mathbf{L}}^n = \mathcal{V}_{2n} = \mathcal{A}_n = \mathcal{B}_n \subset \mathcal{B}_{n-1} \subseteq \mathcal{F}_{n-1}.$$

The limits in the description of \mathcal{B}_{n-1} exist, and are finite, by Theorem 2.4.4. The inclusion $\mathcal{B}_n \subset \mathcal{B}_{n-1}$ can be shown using Green's formula. Consequently, $f \in \mathcal{B}_n$ implies that $\lim_{x \rightarrow b^-} (a_i(x)f^{(i)}(x))^{(i-1)} - \lim_{x \rightarrow a^+} (a_i(x)f^{(i)}(x))^{(i-1)} = 0, \forall i = 1, \dots, n-1$.

Furthermore, the definition of \mathcal{B}_n includes the condition $[f, P_0]_n|_a^b = [f, 1]_n|_a^b = 0$. Hence, the only nonzero terms in equation (3.4.1) are when $j = 1$, yielding n terms. The first $n - 1$ of these terms are precisely those given in the definition of \mathcal{F}_{n-1} , explicitly:

$$\begin{aligned} 0 &= [f, 1]_n|_a^b = \lim_{x \rightarrow b^-} [-a_1 f' + (a_2 f'')' - \dots + (-1)^n (a_n f^{(n)})^{(n-1)}] \\ &\quad - \lim_{x \rightarrow a^+} [-a_1 f' + (a_2 f'')' - \dots + (-1)^n (a_n f^{(n)})^{(n-1)}] \\ &= \lim_{x \rightarrow b^-} (a_n f^{(n)})^{(n-1)} - \lim_{x \rightarrow a^+} (a_n f^{(n)})^{(n-1)}. \end{aligned}$$

Hence also the last condition in \mathcal{F}_n is satisfied, and thus $f \in \mathcal{F}_n$. The claim that $\mathcal{B}_n \subseteq \mathcal{F}_n$ follows by induction on n .

In the induction step, also, any term involving q cancels out. \square

For the reverse inclusion, the proof will involve working with the sesquilinear form explicitly. Hence, the differences between Sturm–Liouville operators arise primarily in the definition of the $a_k(x)$'s in equation (3.4.1). The following theorem is formulated for the Legendre operator.

Theorem 3.4.3. *Let the hypotheses of Conjecture 3.4.1 hold, where ℓ^n is the classical Legendre differential expression given in (3.2.1). Assume that for all $f \in \mathcal{F}_n$, $f'', \dots, f^{(2n-2)} \in L^2[(-1, 1), dx]$. Then we have $\mathcal{F}_n \subseteq \mathcal{C}_n \subseteq \mathcal{B}_n \forall n \in \mathbb{N}$.*

Proof. Fix $n \in \mathbb{N}$. The differential expression ℓ^n can be written in Lagrangian symmetric form as

$$\ell^n[f](x) = \sum_{k=1}^n (-1)^k \left\{ \begin{matrix} n \\ k \end{matrix} \right\}_2 ((1-x^2)^k f^{(k)}(x))^{(k)}, \quad (3.4.2)$$

where $\{n\}_2$ denote the Legendre–Stirling numbers of the second kind, see [6] for more. Hence, $a_k(x) = C(n, k)(1-x^2)^k$, where $C(n, k)$ is a constant. Deconstruct the explicit expression for $[f, P_s]_n|_{-1}^1$ into the following:

$$\begin{aligned} LHS &= \sum_{k=1}^n \sum_{j=1}^k (-1)^{k+j} [a_k(x) P_s^{(k)}(x)]^{(k-j)} f^{(j-1)}(x), \\ RHS &= \sum_{k=1}^n \sum_{j=1}^k (-1)^{k+j+1} [a_k(x) f^{(k)}(x)]^{(k-j)} P_s^{(j-1)}(x). \end{aligned}$$

Assume that $s \geq n$ so that all terms are nonzero. The case where $s < n$ will immediately follow. The assumption that $f \in \mathcal{F}_n$ means that

$$\lim_{x \rightarrow 1^-} [a_k(x) f^{(k)}(x)]^{(k-1)} - \lim_{x \rightarrow -1^+} [a_k(x) f^{(k)}(x)]^{(k-1)} = 0,$$

for $k = 1, \dots, n$, so terms of this form in the RHS will not be of concern. At a single endpoint, consider limits of the form

$$\lim_{x \rightarrow -1^+ \text{ (or } 1^-)} [a_k(x) f^{(k)}(x)]^{(k-2)},$$

for $k = 2, \dots, n$. Assume $c_2 \neq 0$. Without loss of generality, assume that at the endpoint 1 the above limit is equal to $c_2 > 0$ and is finite. Define $r_2 := c_2/2$. Then

$$r_2 < \lim_{x \rightarrow 1^-} [a_k(x) f^{(k)}(x)]^{(k-2)} = \lim_{x \rightarrow 1^-} \left(\sum_{i=0}^{k-2} \binom{k-2}{i} a_k^{(k-2-i)}(x) f^{(k+i)}(x) \right).$$

Recall that $a_k(x) = C(n, k)(1-x^2)^k$, so each term on the right hand side will possess a factor of $(1-x^2)^2$ after differentiation. Dividing both sides by this factor yields

$$\lim_{x \rightarrow 1^-} \frac{r_2}{(1-x^2)^2} < \lim_{x \rightarrow 1^-} \left(\sum_{i=0}^{k-2} \binom{k-2}{i} \tilde{a}_k^{(k-2-i)}(x) f^{(k+i)}(x) \right) =: S_2, \quad (3.4.3)$$

where we use

$$\tilde{a}_k^{(k-2-i)}(x) = \frac{a_k^{(k-2-i)}(x)}{(1-x^2)^2}.$$

Note $k \geq 2$ necessarily here. Hence, the relevant derivatives of $f(x)$ in S_2 are $f''(x), \dots, f^{(n-2)}(x)$, which are all in $L^2[(-1, 1), dx]$ by assumption. However, the

functions $(1 - x^2)^k \in L^2[(-1, 1), dx]$ for all $k \in \mathbb{N}_0$, and so are its derivatives because they are all polynomials. Hence, each summand in S_2 is in $L^1[(-1, 1), dx]$ by the Cauchy–Schwarz inequality, and the finite sum S_2 is then also in $L^1[(-1, 1), dx]$. It is apparent that

$$\lim_{x \rightarrow 1^-} \frac{r_2}{(1 - x^2)^2} = \infty.$$

The comparison test thus yields a contradiction to the fact that $S_2 \in L^1[(-1, 1), dx]$.

As $c_2 \neq 0$ was arbitrary, we conclude

$$\lim_{x \rightarrow 1^-} [a_k(x) f^{(k)}(x)]^{(k-2)} = 0.$$

A similar argument shows that the same result at the endpoint -1 . The method outlined above can be used to show *mutatis mutandis* that

$$\lim_{x \rightarrow 1^-} [a_k(x) f^{(k)}]^{(k-j)} = 0$$

for $2 < j \leq n$. The eigenfunctions $P_s(x)$ are assumed to be polynomials so we may write $P_s(x) = \sum_{h=0}^s \alpha_h x^h$. Then the RHS can be broken down into a power of x times the above limit for each value of $k, j < m$. Basic limit laws say that, for $h \in \mathbb{N}$,

$$\lim_{x \rightarrow 1^-} [a_k(x) f^{(k)}]^{(k-j)} P_s(x) = \sum_{h=0}^s \left(\lim_{x \rightarrow 1^-} \alpha_h x^h [a_k(x) f^{(k)}]^{(k-j)} \right) = 0,$$

by splitting up the product and using the fact that -1 and 1 are finite endpoints.

This means

$$RHS = \sum_{k=1}^n \sum_{j=1}^k (-1)^{k+j+1} [a_k(x) f^{(k)}(x)]^{(k-j)} P_s^{(j-1)}(x) = 0$$

for any $s \in \mathbb{N}$. Likewise,

$$LHS = \sum_{k=1}^n \sum_{j=1}^k (-1)^{k+j} [a_k(x) P_s^{(k)}(x)]^{(k-j)} f^{(j-1)}(x) = 0.$$

The theorem now follows, as this collectively shows $[f, P_s]_n|_{-1}^1 = 0$, for $s \in \mathbb{N}$. \square

The method of proof developed above applies to more than just the Legendre differential expression, with minimal alterations.

Theorem 3.4.4. *Let the hypotheses of Conjecture 3.4.1 hold, where ℓ^n is a classical Jacobi or Laguerre differential expression with $\alpha, \beta > -1$ or $\alpha > -1$ respectively. Assume that for all $f \in \mathcal{F}_n$, $f'', \dots, f^{(2n-2)} \in L^2[(a, b), dx]$. Then we have $\mathcal{F}_n \subseteq \mathcal{C}_n \subseteq \mathcal{B}_n \forall n \in \mathbb{N}$.*

Proof. Fix $n \in \mathbb{N}$. The Jacobi differential expression ℓ_J^n can be written in Lagrangian symmetric form as

$$\ell_J^n[f](x) = \frac{1}{(1-x)^\alpha(1+x)^\beta} \sum_{k=1}^n (-1)^k (C(n, k, \alpha, \beta) (1-x)^{\alpha+k} (1+x)^{\beta+k} f^{(k)}(x))^{(k)},$$

where $C(n, k, \alpha, \beta)$ is a constant, and $\alpha, \beta > -1$. The above proof carries through the same as above, as the term divided through in analogy to equation (3.4.3) will be $(1-x)^{\alpha+2}(1+x)^{\beta+2}$, and has adequate singularities at the endpoints.

The Laguerre differential expression ℓ_L^n can be written in Lagrangian symmetric form as

$$\ell_L^n[f](x) = \frac{1}{x^\alpha e^{-x}} \sum_{k=1}^n (-1)^k (C(n, k, \alpha) x^{\alpha+k} e^{-x} f^{(k)}(x))^{(k)},$$

where $C(n, k, \alpha)$ is a constant, and $\alpha > -1$. The term divided through in analogy to equation (3.4.3) will be $x^{\alpha+2}$, and has an adequate singularity at 0.

More details concerning the setup and properties of these differential equations can be found in [20, 23]. □

This effectively covers most of the classical differential equations which possess complete sets of orthogonal polynomial eigenfunctions. The Hermite equation was not discussed because it does not require boundary conditions of the above forms, as it is limit-point at both $-\infty$ and ∞ .

The astute reader may have noticed that the explicit conditions of \mathcal{F}_n did not play a large part in the above proofs. Indeed, the limit conditions in the definition of \mathcal{F}_n are necessary to prove the assumption that $f'', \dots, f^{(2n-2)} \in L^2[(a, b), dx]$, which was essential. This implication can be accomplished using an appropriate choice of

the vectors ψ and φ in two applications of the so-called CHEL Theorem [52, Theorem 8.7], and subtracting them to form coupled boundary conditions. The limit conditions of \mathcal{F}_n arise as boundary terms from integrating ℓ^n in Lagrangian symmetric form, and can be used to show certain functions are in $L^2[(a, b), dx]$.

It is also important to note that the specific choice of limits in \mathcal{F}_n cannot be altered. Together, they ensure that $[f, P_0]_n|_a^b = [f, 1]_n|_a^b = 0$. The function 1 also happens to be included in every classical orthogonal polynomial sequence so it is particularly applicable.

Finally, with these few extra assumptions, Conjecture 3.4.1 has been shown.

Theorem 3.4.5. Assume the hypotheses of Conjecture 3.4.1, where ℓ^n is a classical Jacobi or Laguerre differential expression, with $\alpha, \beta > -1$ or $\alpha > -1$ respectively. Assume $\mathcal{A}_n = \mathcal{B}_n$ and that $f \in \mathcal{F}_n$ implies that $f'', \dots, f^{(2n-2)} \in L^2[(a, b), dx]$. Then $\mathcal{A}_n = \mathcal{B}_n = \mathcal{C}_n = \mathcal{F}_n = \mathcal{D}_{\mathbf{L}}^n \forall n \in \mathbb{N}$.

CHAPTER FOUR

Iterated Perturbations and Anderson Localization

This chapter partially follows the in-progress manuscript [26], where countably many rank-one perturbations are successively applied to a self-adjoint operator, T , with only absolutely continuous spectrum on a separable Hilbert space \mathcal{H} . Specifically, we utilize the Aronszajn–Donoghue theory to determine that the absolutely continuous spectrum decays with each perturbation, and explicitly compute formulas describing how the initial spectrum changes after an infinite number of such perturbations. This construction involves a curious choice of the perturbation vector at each step in order to control properties of the perturbed operators in terms of the initial operator. In the limiting case, the infinitely perturbed operator is very similar to an Anderson-type Hamiltonian and can be compared to the discrete random Schrödinger operator.

In 1958 P.W. Anderson (Chapter 1, [5]) suggested that sufficiently large impurities in a semi-conductor could lead to spatial localization of electrons, called Anderson localization. The field has grown into a rich theory and is studied by both the physics and the mathematics community. There are many well-studied and famous open problems in this research area, one of which is the Anderson localization conjecture for weak disorder [5,15,69] (or the delocalization conjecture [45]). Here, the existence of *extended states* is defined as non-trivial absolutely continuous spectrum, sometimes referred to as spectral delocalization, in the Anderson-type Hamiltonian. Spectral localization thus refers to an Anderson-type Hamiltonian with trivial absolutely continuous spectrum. However, there are many other definitions of extended states throughout the literature. Section 2.5 describes the setup of Anderson-type Hamiltonians and Kolmogorov’s 0-1 Law.

A primary development is the explicit calculation of the remaining absolutely continuous spectrum after an infinite number of rank-one perturbations. As suggested by Example 4.1.1 below, results for even rank-two perturbations are much more challenging to produce and tend to be less explicit than those for rank-one perturbations. We provide results with Rademacher potential to represent a worst-case scenario for the choice of the sequence of perturbations.

There are several differences between the construction in the current project and classical Anderson-type Hamiltonians:

- (1) The iterative construction requires knowledge of the previous perturbation vector, φ_{n-1} , to choose the next perturbation vector, φ_n . This is very different from Anderson-type Hamiltonians, where the φ_j 's are a sequence of unit vectors chosen a priori, independently from the particular realization of the Anderson-type Hamiltonian. While our limiting operator is very similar to an Anderson-type Hamiltonian, it cannot be explicitly classified as such. Probability measures can be handled in the calculations when Rademacher potentials are considered. As these cases are closer to Anderson-type Hamiltonians in this regard, they are emphasized in Subsection 4.3.3.
- (2) We start on the spectral representation side of the operator. Hence, all of Lebesgue theory can be utilized as a tool, and rank-one perturbation theory becomes more concrete. These tools allow the iterative introduction of infinitely many rank-one perturbations, and the resulting operator is similar to an Anderson-type Hamiltonian.
- (3) The construction yields an operator of spectral multiplicity one. A general Anderson-type Hamiltonian does not necessarily possess spectral multiplicity one.

The main tools of perturbation theory from Section 2.1 are utilized in Section 4.1, where the majority of preparatory calculations take place, including applying

Aronszajn–Donoghue theory to the first perturbation. Beginning with a measure that is constant over the interval $[-1, 1]$, Aronszajn–Donoghue theory says that a perturbation creates a point mass outside of $[-1, 1]$ and the remaining absolutely continuous spectrum is reduced accordingly. The precise strength of the point mass is calculated, and although it is possible to explicitly find a formula for the absolutely continuous spectral measure, it is avoided here for simplicity. Subsection 4.1.1 represents a comparison for the level of difficulty involved in computing even a rank-two perturbation. Recent developments in finite rank perturbations can be found, for example, in [36, 44, 46].

Section 4.2 explains the techniques involved in the iterative construction. Specifically, choosing the second perturbation vector $\tilde{\varphi}_2$ allows us to pass via unitary equivalence from the often byzantine a.c. spectral measure on $[-1, 1]$ to an auxiliary measure that is simply a constant on $[-1, 1]$ again. We are mainly concerned with the total mass (or total variation) of the a.c. part of this auxiliary measure. This auxiliary measure is comparable to the beginning measure and is unchanged through the spectral theorem and the unitary operator. This unitary operator and choice of the vector $\tilde{\varphi}_2$ return us to the situation at the beginning of Section 4.1, with a constant measure on $[-1, 1]$.

Section 4.3 iterates this utilization of vector choices and unitary operators along with the perturbations. New perturbations are orthogonal to the point masses created from previous ones and therefore can be avoided; this allows us to focus on the absolutely continuous spectrum. Formulas that are similar to those from Section 4.2 are produced and the process can effectively be iterated. The final formulas obtained from iteration are found in Subsections 4.3.1 and 4.3.2. Subsection 4.3.3 then draws conclusions from these formulas. Specifically, the constructed operator with Rademacher potential, where the α 's are chosen at the endpoints of the given

interval, is found to have spectral localization. These formulas are quite simple and shed light onto the recursive nature of the process.

Section 4.4 attempts to escape the requirement of the previous construction of orthogonal perturbation vectors, and obtains results for how much absolutely continuous spectrum can be destroyed via a single rank-one perturbation. These estimates are upper-bounds and require knowledge of how the perturbation vector interacts with the spectral measure. The goal is to bring the constructed operator closer to being an Anderson-type Hamiltonian by allowing more freedom for the choices of the vectors. Unfortunately, the estimates obtained are not sharp enough to iterate using the devised methods and further refinement is still required. However, the estimates are the first known of their kind for general perturbation theory and are of interest for those purposes as well. The methods used rely on an intimate knowledge of Aronszajn–Donoghue theory and the integral transforms involved within.

4.1 A First Perturbation

Consider a self-adjoint operator T on a separable Hilbert space \mathcal{H} . Without loss of generality, it is assumed that T is cyclic with cyclic vector φ , i.e. satisfies equation (2.1.2). The formal expression for the rank-one perturbation of the operator T is written as

$$H_{\alpha_1} = T + \alpha_1 \langle \cdot, \varphi \rangle_{\mathcal{H}} \varphi \quad \text{for} \quad \alpha_1 \in \mathbb{R},$$

as described in Section 2.1. The spectral theorem can now be applied to obtain the spectral representation

$$\tilde{H}_{\alpha_1} = M_t + \alpha_1 \langle \cdot, \tilde{\varphi}_1 \rangle_{L^2(\tilde{\mu}_0)} \tilde{\varphi}_1 \quad \text{on} \quad L^2(\tilde{\mu}_0), \quad (4.1.1)$$

where the vector $\tilde{\varphi}_1 \equiv \text{constant}$. The spectral measure of the unperturbed operator T is chosen to be

$$d\tilde{\mu}_0 := \frac{1}{2} \chi_{[-1,1]} dx. \quad (4.1.2)$$

This measure is, without loss of generality, chosen as an example of the general process only to simplify calculations. Indeed, one of the main advances from this Chapter is that if $\tilde{\mu}_0$ is absolutely continuous and given by some other weight function on $[-1, 1]$, the process from Section 4.2 can be applied to yield a unitarily equivalent constant measure on $[-1, 1]$ instead. Also, without loss of generality we assume $\tilde{\varphi}_1$ has norm 1, so that

$$\tilde{\varphi}_1 \equiv \mathbf{1}.$$

It is now necessary to introduce some manner of comparing the strength of spectral measures in order to track their overall growth or decay as more rank-one perturbations are applied. For this purpose, we choose to study the norm, or total mass, of the absolutely continuous part of the produced spectral measures. The norm of a measure η over the real line will be denoted by

$$\|\eta\| := \int_{\mathbb{R}} d\eta(t).$$

These initial assumptions have been set up so that $\|\tilde{\mu}_0\| = 1$ by construction. The perturbed operator can be thoroughly examined using Aronszajn–Donoghue Theory, specifically Theorem 2.1.2. Most of the final results will come by generalizing the following computations and making specific choices of the perturbation vectors and unitary operators.

Lemma 4.1.1. Let \tilde{H}_{α_1} and $\tilde{\mu}_0$ be given by Equations (4.1.1) and (4.1.2) respectively. If $\alpha_1 \neq 0$, then the following statements hold:

(1) \tilde{H}_{α_1} has an eigenvalue at

$$x_{\alpha_1} := \frac{-1 - e^{2/\alpha_1}}{1 - e^{2/\alpha_1}},$$

Furthermore, the eigenvalue x_{α_1} falls outside of the interval $[-1, 1]$, regardless of the choice of α_1 .

(2) Let μ_{α_1} be the spectral measure of \tilde{H}_{α_1} . Then the weight of the created eigenvalue is

$$\mu_{\alpha_1}\{x_{\alpha_1}\} = \frac{4e^{2/\alpha_1}}{\alpha_1^2(e^{2/\alpha_1} - 1)^2}.$$

Proof. (1) Begin by observing that for all $x \notin [-1, 1]$ we have

$$G(x) = \int_{-1}^1 \frac{d\tilde{\mu}_0(\lambda)}{(\lambda - x)^2} < \infty.$$

Theorem 2.1.2 then says that

$$\tilde{H}_{\alpha_1} \text{ has an eigenvalue at } x \notin [-1, 1] \iff -\frac{1}{\alpha_1} = F(x + i0),$$

where $F(z) = \int_{\mathbb{R}} \frac{d\tilde{\mu}_0(\lambda)}{\lambda - z}$. The equation on the right side of the implication is now made explicit for $x \notin [-1, 1]$ as

$$-\frac{1}{\alpha_1} = \int_{\mathbb{R}} \frac{d\tilde{\mu}_0(\lambda)}{\lambda - x} = \frac{1}{2} \int_{-1}^1 \frac{d\lambda}{\lambda - x} = \frac{1}{2} \ln \left(\frac{1 - x}{-1 - x} \right)$$

The solution to the previous equation for x depends on α_1 and will be denoted as

$$x_{\alpha_1} := \frac{-1 - e^{2/\alpha_1}}{1 - e^{2/\alpha_1}}.$$

In particular, $x_{\alpha_1} < -1$ for $\alpha_1 < 0$, while $x_{\alpha_1} > 1$ for $\alpha_1 > 0$.

(2) Let μ_{α_1} denote the spectral measure of \tilde{H}_{α_1} . The mass of the created eigenvalue is now given by Theorem 2.1.2:

$$\mu_{\alpha_1}\{x_{\alpha_1}\} = \frac{1}{\alpha_1^2 G(x_{\alpha_1})}.$$

The value of the integral transform in the denominator can be calculated as

$$G(x_{\alpha_1}) = \frac{1}{2} \int_{-1}^1 \frac{d\lambda}{(\lambda - x_{\alpha_1})^2} = -\frac{1}{2} \left[\frac{1}{1 - x_{\alpha_1}} + \frac{1}{1 + x_{\alpha_1}} \right].$$

Inserting the value of x_{α_1} given in (1) yields $1/G(x_{\alpha_1}) = \frac{4e^{2/\alpha_1}}{(e^{2/\alpha_1} - 1)^2}$. Finally,

$$\mu_{\alpha_1}\{x_{\alpha_1}\} = \frac{4e^{2/\alpha_1}}{\alpha_1^2(e^{2/\alpha_1} - 1)^2}.$$

This completes the proof. □

4.1.1 Motivational Rank-Two Example

In order to grasp the difficulty of computing the absolutely continuous part of the spectrum for even a rank-two perturbation, without using the methods developed in this Chapter, we offer an illustrative example. Without loss of generality we consider this rank-two problem in the spectral representation with respect to one of the two perturbation vectors. That is, let us take the spectral measure of the unperturbed self-adjoint operator T to be (as above) $d\mu := \frac{1}{2}\chi_{[-1,1]}dx$, and consider the normalized vectors $\varphi_1, \varphi_2 \in L^2(\mu)$.

The rank-two perturbation is then written as

$$H_{\alpha,\beta} = M_t + \alpha \langle \cdot, \varphi_1 \rangle_{L^2(\mu)} \varphi_1 + \beta \langle \cdot, \varphi_2 \rangle_{L^2(\mu)} \varphi_2 \quad \text{on} \quad L^2(\mu).$$

Aronszajn–Donoghue theory can be applied to compute the absolutely continuous part of the rank-one perturbation $H_{\alpha,0}$:

$$d[(\mu_{\alpha,0})_{ac}](x) = \frac{1}{2} \left\{ 1 + \alpha^2 + \alpha \ln \left(\frac{x+1}{-x+1} \right) + \left(\frac{\alpha}{4} \right)^2 \left[\ln \left(\frac{x+1}{-x+1} \right) \right]^2 \right\}^{-1} dx \quad (4.1.3)$$

for $x \in [-1, 1]$, and $(\mu_{\alpha,0})_{ac} \equiv 0$ outside $[-1, 1]$. The introduction of the second rank-one perturbation to the problem leaves the new spectral measure quite expensive to compute, even with the use of Mathematica. Indeed, Aronszajn–Donoghue theory will require integration with respect to $\mu_{\alpha,0}$. As a consequence, computing the eigenvalues under such an iterative rank-two perturbation seems practically unfeasible. The introduction of further perturbations would only serve to complicate matters further.

4.2 Constructing the Iterated Operator

This section explains the heart of our construction by describing how a rank-one perturbation is extended to a rank-two perturbation. The choice of the direction of the second perturbation, φ_2 , plays a key role and allows us to calculate the norm of the remaining absolutely continuous part of the spectrum. The difficulties encountered

in the previous example are bypassed by applying a unitary transformation which exploits the choice of φ_2 . After the transformation, computations from Aronszajn–Donoghue theory again resemble those of Lemma 4.1.1.

Recall the rank-one perturbation setup discussed in Section 4.1 above. Namely,

$$\tilde{H}_{\alpha_1} = M_t + \alpha_1 \langle \cdot, \tilde{\varphi}_1 \rangle_{L^2(\tilde{\mu}_0)} \tilde{\varphi}_1 \text{ on } L^2(\tilde{\mu}_0) \text{ where } d\tilde{\mu}_0 := \frac{1}{2} \chi_{[-1,1]} dx \text{ and } \tilde{\varphi}_1 \equiv \mathbf{1}.$$

Aronszajn–Donoghue Theory (Theorem 2.1.2) has provided us with information about the spectral measure, μ_{α_1} , of the perturbed operator \tilde{H}_{α_1} in the previous Section. Furthermore, we know that the support of the absolutely continuous part of the measure is still equal to $[-1, 1]$ due to the Kato–Rosenblum Theorem 2.1.4. The operator \tilde{H}_{α_1} is represented in the space $L^2(\mu_{\alpha_1})$ as multiplication by the independent variable due to the spectral theorem.

By a slight abuse of notation, for future iterations we will still write M_t for this operator to avoid an infinite sequence of independent variables. In particular, we have the unitary equivalence between operators

$$\left(\tilde{H}_{\alpha_1} \text{ on } L^2(\tilde{\mu}_0) \right) \sim \left(M_t \text{ on } L^2(\mu_{\alpha_1}) \right).$$

Let $V_{\alpha_1} : L^2(\tilde{\mu}_0) \rightarrow L^2(\mu_{\alpha_1})$ denote this intertwining unitary operator such that

$$V_{\alpha_1} \tilde{H}_{\alpha_1} = M_t V_{\alpha_1} \quad \text{and} \quad V_{\alpha_1} \tilde{\varphi}_1 \equiv \text{constant}.$$

Of course, the value of the constant can be determined by normalizing $V_{\alpha_1} \tilde{\varphi}_1$. The operator V_{α_1} is given explicitly in the Representation Theorem 2.1.1 [47]. Hence, by construction we have that $V_{\alpha_1} \mathbf{1} = \mathbf{1}$, where the $\mathbf{1}$ vectors are understood to be in the appropriate L^2 spaces, $L^2(\tilde{\mu}_0)$ and $L^2(\mu_{\alpha_1})$ respectively. Indeed, the unitary property of V_{α_1} provides the following string of equalities:

$$\begin{aligned} \|\tilde{\mu}_0\| &= \int_{\mathbb{R}} d\tilde{\mu}_0(t) = \int_{\mathbb{R}} \mathbf{1} d\tilde{\mu}_0(t) = \|\mathbf{1}\|_{L^2(\tilde{\mu}_0)} = \|V_{\alpha_1} \mathbf{1}\|_{L^2(\mu_{\alpha_1})} \\ &= \|\mathbf{1}\|_{L^2(\mu_{\alpha_1})} = \int_{\mathbb{R}} \mathbf{1} d\mu_{\alpha_1}(t) = \int_{\mathbb{R}} d\mu_{\alpha_1}(t) = \|\mu_{\alpha_1}\|. \end{aligned}$$

Remark. Researchers experienced in the field may feel this previous calculation to be contradictory to results in Clark theory, the basis of unitary rank-one perturbation theory. However, a central theme discovered while producing these results is that self-adjoint theory and unitary theory are quite different. For instance, attempting to move this calculation into the unitary perturbation case with the Cayley Transform involves an adjustment for the perturbation vector which causes some cancellations, see [48, Lemma 5.1]. Furthermore, the condition in the Representation Theorem that requires $V_{\alpha_1} \mathbf{1} = \mathbf{1}$ is believed to be equivalent to the statement that $\theta(0) = 0$, where θ is the generating characteristic function for the Clark measures. Hence, a contradiction with a result similar to [14, Prop. 9.1.8] is not created.

The second rank-one perturbation is now added in the direction of some particular function $\varphi_2 \in \mathcal{H}$. The task will now be to consider

$$H_{\alpha_2} = M_t + \alpha_2 \langle \cdot, \varphi_2 \rangle_{L^2(\mu_{\alpha_1})} \varphi_2 \quad \text{on } L^2(\mu_{\alpha_1}). \quad (4.2.1)$$

The following proposition encapsulates the main idea of this work: the choice of φ_2 and of the unitary operator U_1 which passes the spectral calculations from $L^2(\mu_{\alpha_1})$ to an *auxiliary space* denoted by $L^2(\tilde{\mu}_{\alpha_1})$. The problem is thus simplified to one that resembles the setup in Section 4.1.

Proposition 4.2.1. *The rank-two perturbation \tilde{H}_{α_2} can be recast as*

$$\tilde{H}_{\alpha_2} = M_t + \alpha_2 \langle \cdot, \tilde{\varphi}_2 \rangle_{L^2(\tilde{\mu}_{\alpha_1})} \tilde{\varphi}_2 \quad \text{on } L^2(\tilde{\mu}_{\alpha_1}). \quad (4.2.2)$$

By a choice of a unit vector $\varphi_2 \in L^2(\mu_{\alpha_1})$ and a unitary multiplication operator U_1 , we can arrange for

- (1) $d(\tilde{\mu}_{\alpha_1})_{ac} = \tau_1 \chi_{[-1,1]} dx$ for some constant τ_1 ,
- (2) $\varphi_2 \perp L^2[(\mu_{\alpha_1})_{pp}]$, and
- (3) $\varphi_2 \perp \mathbf{1}$ (recall that $V_{\alpha_1} \tilde{\varphi}_1 \equiv \text{constant}$, so that $\varphi_2 \perp V_{\alpha_1} \tilde{\varphi}_1$).

Before we prove this proposition we observe that the mass of the absolutely continuous part of the first spectral measure was 1, i.e. $\|(\tilde{\mu}_0)_{ac}\| = 1$. Future iterations will not have this property. For instance, let $(\mu_{\alpha_2})_{ac}$ denote the absolutely continuous part of the spectral measure corresponding to the rank-two perturbed operator \tilde{H}_{α_2} . In light of the above discussion on the properties of V_{α_1} , the mass of this measure can be calculated as

$$\|(\mu_{\alpha_2})_{ac}\| = \|(\mu_{\alpha_1})_{ac}\| - \mu_{\alpha_1}\{x_{\alpha_1}\} \neq 1.$$

However, the calculation of $\|(\mu_{\alpha_1})_{ac}\|$ is in general quite difficult, as shown in the Example of Subsection 4.1.1. The task becomes much simpler, according to the Proposition, when we pass to an auxiliary measure $\tilde{\mu}_{\alpha_1}$. Indeed, the numerical constant τ_1 is related to those in Lemma 4.1.1 via $\tau_1 = \|(\tilde{\mu}_{\alpha_1})_{ac}\|/2$.

Proof of Proposition 4.2.1. Assume that $\text{supp } \varphi_2 \subset [-1, 1]$. This assumption will be made concrete later when a specific choice for φ_2 is made. Recall that x_{α_1} was an eigenvalue outside $[-1, 1]$ created by φ_1 , analyzed in Lemma 4.1.1. The corresponding eigenvector is supported at the single point $\{x_{\alpha_1}\}$. Therefore, $\varphi_2 \perp L^2[(\mu_{\alpha_1})_{pp}]$ and x_{α_1} will remain unchanged by the second perturbation. Moreover, the operator decomposes into the orthogonal sum

$$H_{\alpha_2} = M_t \oplus [M_t + \alpha_2 \langle \cdot, \varphi_2 \rangle_{L^2(\mu_{\alpha_1})} \varphi_2] \quad \text{on } L^2[(\mu_{\alpha_1})_{pp}] \oplus L^2[(\mu_{\alpha_1})_{ac}], \quad (4.2.3)$$

and we reduce further examinations to $M_t + \alpha_2 \langle \cdot, \varphi_2 \rangle \varphi_2$ on $L^2[(\mu_{\alpha_1})_{ac}]$. We translate this operator into an auxiliary space by choosing an appropriate unitary multiplication operator, denoted U_1 , so that $M_t + \alpha_2 \langle \cdot, \varphi_2 \rangle \varphi_2$ on $L^2[(\mu_{\alpha_1})_{ac}]$ is unitarily equivalent to equation (4.2.2).

The first perturbation only had the effect of creating an eigenvalue, so we may assume that

$$d(\mu_{\alpha_1})_{ac} = w_1(t)dt,$$

where $w_1(t)$ is some weight function. This weight function can be exactly determined by using Theorem 2.1.2 and Lemma 2.1.3, and is stated in Subsection 4.1.1, but we omit this very tedious calculation for brevity. However, if we consider the previous weight function for $\tilde{\mu}_0$, which is $w_0(t) = 1/2\chi_{[-1,1]}$, we can see that by Theorem 2.1.4 (Kato–Rosenblum) the weight $w_1(t)$ is unitarily equivalent to $w_0(t)$. This means that

$$w_1, \frac{1}{w_1} \in L^1_{loc}[-1, 1].$$

In particular, take $U_1 : L^2[(\mu_{\alpha_1})_{ac}] \rightarrow L^2(\tilde{\mu}_{\alpha_1})$ to be

$$U_1 := M_{\sqrt{w_1(t)/h_2(t)}} \quad (4.2.4)$$

where $|h_2| = 1$ with details determined at the end of this proof. It is important to note that U_1 is unitary: if $f \in L^2(\mu_{\alpha_1})_{ac}$, then

$$\begin{aligned} \|f\|_{L^2[(\mu_{\alpha_1})_{ac}]}^2 &= \int_{-1}^1 |f(t)|^2 d(\mu_{\alpha_1})_{ac} = \int_{-1}^1 |f(t)|^2 w_1(t) dt \\ &= \int_{-1}^1 |f(t) \sqrt{w_1(t)}|^2 dt = \|\sqrt{w_1(t)} f\|_{L^2(\tilde{\mu}_{\alpha_1})}^2 = \|U_1 f\|_{L^2(\tilde{\mu}_{\alpha_1})}^2. \end{aligned}$$

The trick is now to choose φ_2 in a particular way in order to ultimately achieve

$$d(\tilde{\mu}_{\alpha_1})_{ac} \equiv \tau_1 \chi_{[-1,1]} dx \equiv (\text{const.}) d\tilde{\mu}_0.$$

This will allow us to repeat the iteration process as many times as desired. The operator U_1 determines $\tilde{\varphi}_2 = \sqrt{w_1(t)} \varphi_2$ from our previous discussion, and the total mass of $\tilde{\mu}_{\alpha_1}$ should remain 1.

We need $\tilde{\varphi}_2$ to be a unit vector in $L^2(\tilde{\mu}_1)$. Hence,

$$\begin{aligned} 1 = \|\tilde{\varphi}_2\|_{L^2(\tilde{\mu}_{\alpha_1})}^2 &= \int_{-1}^1 |\tilde{\varphi}_2|^2 d\tilde{\mu}_{\alpha_1} = \int_{-1}^1 |U_1 \varphi_2|^2 d\tilde{\mu}_{\alpha_1} \\ &= \int_{-1}^1 |\varphi_2|^2 d\mu_{\alpha_1} = \int_{-1}^1 |\varphi_2|^2 w_1(t) dt. \end{aligned}$$

Therefore, the choice

$$\varphi_2(t) = \begin{cases} \frac{h_2(t)}{\sqrt{2w_1(t)}} & \text{for } t \in (-1, 1), \\ 0 & \text{else} \end{cases}$$

yields the desired result. It can be seen that with these choices of U_1 and φ_2 , the spectral theorem implies that τ_1 is indeed a constant.

Finally, h_2 chosen in accordance with Lemma 4.2.3 implies property (3). \square

Corollary 4.2.2. *The value for τ_1 from in (4.2.2) can be explicitly calculated as*

$$\tau_1 = \frac{1}{2} - \frac{2e^{2/\alpha_1}}{\alpha_1^2(e^{2/\alpha_1} - 1)^2}.$$

Proof. Recall that $\tau_1 = \|(\tilde{\mu}_{\alpha_1})_{ac}\|/2$. First notice that we have lost mass inside the interval $[-1, 1]$ due to the eigenvalue created by the first rank-one perturbation. However, in Section 4.1 we explicitly computed the mass of x_{α_1} . This combined with the previous comment that the norm of $\tilde{\mu}_{\alpha_1}$ remains at 1 and the fact that all our operators are unitary, allows us to deduce

$$\tau_1 \int_{-1}^1 dx = \int_{-1}^1 d(\tilde{\mu}_{\alpha_1})_{ac}(x) = 1 - \mu_{\alpha_1}\{x_{\alpha_1}\} = 1 - \frac{4e^{2/\alpha_1}}{\alpha_1^2(e^{2/\alpha_1} - 1)^2}.$$

Multiplying both sides of the equation by $1/2$ yields the desired result. \square

4.2.1 Orthogonality of Perturbations

This elementary proof is included for the convenience of the reader, and is motivated by Theorem 2.10 in [3] and the definition of the Lebesgue integral.

Lemma 4.2.3. *Let $S = \{f_n\}_{n=1}^N$ be a finite set of functions orthogonal in a separable Hilbert space $L^2(\eta)$, where η is a positive Borel measure supported on $[-1, 1]$ without a point mass at $x = 1$. Then for some measurable function $h(x)$, with $|h(x)| = 1$ a.e. with respect to η , the set $S \cup \{h\}$ is orthogonal.*

Proof. Without loss of generality, we consider the positive parts of each f_n , $f_n^+(x) := \max\{f_n(x), 0\}$. Let $\{g_m^n\}_{m \in \mathbb{N}}$ be the sequence of simple functions in standard representation which approximates f_n^+ pointwise and uniformly (wherever f_n^+ is bounded).

Let E_m^n denote the partition of $[-1, 1)$ on which g_m^n is constant. For $n = 1, \dots, N$, take the union of the endpoints of E_m^n and cover $[-1, 1)$ by non-overlapping

half-open intervals corresponding to this union. Denote the collection of these intervals by I_m . Then, for each fixed m , g_m^n , $n = 1, \dots, N$, is constant on each half-open interval $I \subset I_m$.

For each $I \subset I_m$ define

$$h_m|_I = \begin{cases} 0 & \text{on } [-1, 1) \setminus I \\ 1 & \text{on the right half of } I \\ -1 & \text{on the left half of } I \end{cases}$$

and $h_m := \sum_I h_m|_I$. This gives us that $\langle g_m^n, h_m \rangle = 0$, $\forall m, n$, and h_m converges with respect to η to some measurable h with $|h(x)| = 1$ on $[-1, 1)$.

All that remains to show is that $\langle f_n, h \rangle = 0$, $\forall n$. This follows by a simple application of the Dominated Convergence Theorem to the functions $g_m^n(x)$ and $h(x)$:

$$\begin{aligned} \langle f_n, h \rangle &= \int_{-1}^1 \lim_{m \rightarrow \infty} g_m^n(x) h_m(x) d\eta(x) \\ &= \lim_{m \rightarrow \infty} \int_{-1}^1 g_m^n(x) h_m(x) d\eta(x) \\ &= 0 \quad \forall n. \end{aligned}$$

This completes the proof. □

4.3 Infinite Iterations and the Absolutely Continuous Spectrum

The iteration strategy can now be decomposed into the following steps:

- (1) Begin with an unperturbed operator that is multiplication by the independent variable on some $L^2(\mu)$ space. At step k the measure will be given by $\mu_{\alpha_{k-1}}$.
- (2) Perturb the operator by the appropriate vector φ , as explained in Subsection 4.3.1. The choice of α can be done in several different ways, some of which will be discussed in Subsection 4.3.3.
- (3) Apply an appropriate unitary operator (in analogy to the choice in (4.2.4)) to move the operator to an auxiliary space $\tilde{\mu}$, where $d\tilde{\mu} = \tau \chi_{[-1,1]} dx$.

- (4) Determine the relevant constants. Specifically τ , which describes the remaining total mass after the iteration, see Subsection 4.3.2.
- (5) Apply the Spectral Theorem to move to a new L^2 space in which the perturbed operator H_{α_k} is multiplication by the independent variable.
- (6) Return to Step 1.

4.3.1 The k -th Perturbation Vector

After step (1) the problem is to consider the k -th rank-one perturbation. In analogy to equation (4.2.2) we now consider

$$H_{\alpha_k} = M_t + \alpha_k \langle \cdot, \varphi_k \rangle_{L^2(\mu_{\alpha_{k-1}})} \varphi_k \quad \text{on } L^2(\mu_{\alpha_{k-1}}).$$

Let $\{f_1, \dots, f_{k-1}\}$ denote the vectors in $L^2(\mu_{\alpha_{k-1}})$ that correspond to the directions of previous perturbations, which were chosen after the previous $k-1$ steps. In other words, we let

$$\left(f_n \in L^2(\mu_{\alpha_{k-1}}) \right) \sim \left(\varphi_n \in L^2(\mu_{\alpha_n}) \right) \quad \text{for } n = 1, \dots, k-1,$$

where \sim refers to the appropriate composition (different for each n) of unitary transformations. The following Corollary of Proposition 4.2.1 shows that the direction of the k -th perturbation vector φ_k can be chosen analogously.

Corollary 4.3.1. *We can choose the vector $\varphi_k \in L^2(\mu_{\alpha_{k-1}})$ so that the following conditions hold.*

- (1) *The vector $\varphi_k \perp L^2[(\mu_{\alpha_n})_{\text{pp}}]$ for all $n = 1, \dots, k-1$.*
- (2) *The vector $\varphi_k \perp f_n$ for all $n = 1, \dots, k-1$.*
- (3) *The rank- k perturbation of interest becomes*

$$\tilde{H}_{\alpha_k} = M_t + \alpha_k \langle \cdot, \tilde{\varphi}_k \rangle_{L^2(\tilde{\mu}_{\alpha_{k-1}})} \tilde{\varphi}_k \quad \text{on } L^2(\tilde{\mu}_{\alpha_{k-1}}) \tag{4.3.1}$$

$$\text{where } d\tilde{\mu}_{k-1} \equiv \tau_{k-1} \chi_{[-1,1]} dx.$$

Again, recall that M_t in $L^2(\tilde{\mu}_{\alpha_{k-1}})$ corresponds to the previous rank- $(k-1)$ perturbation in its spectral representation.

Proceeding as in Corollary 4.2.2, we note that $\tau_{k-1} = m_{k-1}/2 = \|(\tilde{\mu}_{\alpha_{k-1}})_{ac}\|/2$.

Proof. We mimic the proof of Proposition 4.2.1. Consider

$$\varphi_k(t) := \begin{cases} 0 & \text{on } \mathbb{R} \setminus [-1, 1], \\ \frac{h_k(t)}{\sqrt{2w_{k-1}(t)}} & \text{on } (-1, 1), \end{cases}$$

where $d(\mu_{k-1})_{ac} = w_{k-1}(t)dx$. The function $h_k(t)$ is such that $|h_k(t)| = 1$ on $(-1, 1)$, and is chosen by Lemma 4.2.3 with

$$d\eta = \frac{d\mu_{\alpha_{k-1}}}{\sqrt{2w_{k-1}(t)}}, \quad f_n = f_n(n = 1, \dots, l = k-1), \quad \text{and} \quad h = h_k.$$

This implies that condition (1) holds. Define the multiplication operator $U_{k-1} : L^2[(\mu_{\alpha_{k-1}})_{ac}] \rightarrow L^2(\tilde{\mu}_{k-1})$ to be

$$U_{k-1} := M_{\sqrt{w_{k-1}(t)/h_k(t)}}.$$

If we denote $U_{k-1}\varphi_k$ by $\tilde{\varphi}_k$, we then have that $\|\tilde{\varphi}_k\|_{L^2(\tilde{\mu}_{k-1})} = 1$. Condition (3) is then obtained by the definition of the spectral theorem, as in Proposition 4.2.1.

□

4.3.2 Remaining Absolutely Continuous Spectrum after k Iterations

The desired byproduct of this construction is now achieved. The specific choice of φ_k at each step in Corollary 4.3.1 allows the proof of Lemma 4.1.1 to be generalized to each iteration because

$$G_k(x) = \int_{\mathbb{R}} \frac{d\tilde{\mu}_k(t)}{(t-x)^2} = \tau_k \int_{-1}^1 \frac{dt}{(t-x)^2} < \infty \quad \text{for } x \notin [-1, 1].$$

This means that Aronszajn–Donoghue theory applies and the essential formulas from Section 4.2 can be generalized.

Recall that $d\tilde{\mu}_0 = \tau_0 \chi_{[-1,1]} dx$, with $\tau_0 = 1/2$ as above. In general, by equation (4.3.1) we will have

$$d(\tilde{\mu}_{\alpha_k})_{ac} = \tau_k \chi_{[-1,1]} dx.$$

We determine τ_k in a similar way as τ_1 in Section 4.2. Specifically,

$$\tau_k = \frac{\|(\mu_{\alpha_{k-1}})_{ac}\|}{2} - \frac{\tilde{\mu}_{\alpha_k}\{x_{\alpha_k}\}}{2}.$$

Again, the eigenvalue x_{α_k} , created by the perturbation α_k , is unaffected by subsequent perturbations. However, the calculations for $\tilde{\mu}_{\alpha_k}\{x_{\alpha_k}\}$ will involve the constant τ_{k-1} from the previous step. Hence, the formulas in Section 4.2 are recursive and need to be altered slightly. The relevant calculation is

$$\|(\tilde{\mu}_{\alpha_k})_{ac}\| = \|(\tilde{\mu}_{\alpha_{k-1}})_{ac}\| - \tilde{\mu}_{\alpha_k}\{x_{\alpha_k}\} = 1 - \sum_{n=1}^k \tilde{\mu}_{\alpha_n}\{x_{\alpha_n}\} \quad (4.3.2)$$

$$= 1 - \sum_{n=1}^k \frac{e^{1/\alpha_n \tau_{n-1}}}{\alpha_n^2 \tau_{n-1} (e^{1/\alpha_n \tau_{n-1}} - 1)^2}. \quad (4.3.3)$$

The recursive process used to determine constants for the above calculation can be illustrated as follows:

$$\tau_{k-1} \quad \rightarrow \quad \tilde{\mu}_{\alpha_k}\{x_{\alpha_k}\} \quad \rightarrow \quad \|(\tilde{\mu}_{\alpha_k})_{ac}\| = 2\tau_k$$

Hence τ_k , $k \in \mathbb{N}$, depends on the realization of all previously chosen perturbation parameters $\alpha_1, \alpha_2, \dots, \alpha_k$.

4.3.3 Rademacher Potential

The concepts developed in the previous two Subsections can be applied with different choices of the perturbation parameters. We wish to determine whether certain iterated operators, or classes of them, localize ($\lim_{k \rightarrow \infty} \tau_k = 0$) or delocalize ($\lim_{k \rightarrow \infty} \tau_k > 0$) and what conditions are necessary and/or sufficient for such behavior. It is now clear that much of the previous construction can be easily adapted to various

scenarios, so we make a slightly different choice of our starting measure. Let the starting measure be chosen as $\tilde{\mu}_0 = \frac{1}{2c}\chi_{[-c,c]}dx$. Recall that the choice of a constant function here is possible as long as the beginning weight function is in $L^1_{\text{loc}}(-c, c)$. This is because a unitary operator can then be applied, as described in Section 4.2, to begin with a constant weight function. Hence, the interval of support is more desirable to generalize.

The simplest scenario is to start with the perturbation parameters given by $\{\alpha_n\}_{n=1}^k$ chosen with respect to a Rademacher distribution, i.e. $\alpha_n = \pm c$. These parameters collectively take the place of the potential in the description of Anderson-type Hamiltonians, and in particular the discrete Schrödinger operator, described in Section 2.5. Consequently, we refer to the choice of $\alpha_n = \pm c$, $n = 1, \dots, k$, as defining a Rademacher potential.

Theorem 4.3.2. The operator constructed in the previous three sections, when the $\{\alpha_k\}$'s are chosen i.i.d. with respect to the probability measure $\mathbb{P} = \frac{1}{2}\delta_{-c} + \frac{1}{2}\delta_c$ (Rademacher potential), localizes for any fixed disorder $c > 0$.

Proof. The equation 4.3.2 can be adjusted to let $\alpha_n = \pm c$ for all n to state:

$$\|(\tilde{\mu}_{\alpha_k})_{ac}\| = 1 - \frac{1}{c^2} \sum_{n=1}^k \frac{e^{1/c\tau_{n-1}}}{\tau_{n-1}(e^{1/c\tau_{n-1}} - 1)^2}.$$

We are mainly concerned with the exact limiting value of this series. The convergence of this series is clear: Physics tells us that the absolutely continuous part of $\tilde{\mu}_{\alpha_k}$ cannot become negative, it is bounded above by 1, and the sequence of partial sums decreases as k increases. The summand can be rearranged by expanding the denominator and factoring out a term of $e^{1/c\tau_{n-1}}$ to yield

$$\frac{e^{1/c\tau_{n-1}}}{\tau_{n-1}(e^{1/c\tau_{n-1}} - 1)^2} = \frac{1}{\tau_{n-1}(e^{1/c\tau_{n-1}} - 2 + e^{-1/c\tau_{n-1}})}.$$

Hence, localization necessitates

$$\lim_{n \rightarrow \infty} [\tau_{n-1}(e^{1/c\tau_{n-1}} - 2 + e^{-1/c\tau_{n-1}})] = \infty.$$

In this specific scenario, the operator began with a total mass of 1. This implies $0 \leq \tau_{n-1} \leq 1$. Hence, for fixed c , we have:

$$\begin{aligned} \lim_{n \rightarrow \infty} [\tau_{n-1}(e^{1/c\tau_{n-1}} - 2 + e^{-1/c\tau_{n-1}})] = \infty &\iff \lim_{n \rightarrow \infty} e^{1/c\tau_{n-1}} = \infty \\ &\iff \lim_{n \rightarrow \infty} \tau_{n-1} = 0 \end{aligned}$$

The first if and only if statement can be verified by noticing that the exponential is “stronger” than the τ_{n-1} term. Also, $e^{-1/c\tau_{n-1}}$ remains bounded for $0 \leq \tau_{n-1} \leq 1$ by $e^{-1/c}$. Therefore, we conclude that if $\tau_{k-1} \not\rightarrow 0$ as $k \rightarrow \infty$, then the sum does not converge. This is a contradiction, so it must be that $\tau_{k-1} \rightarrow 0$ as $k \rightarrow \infty$, and the operator localizes. \square

4.4 Non-Orthogonal Perturbations

We now shift gears from the construction that was the main concern of the previous three Sections, and attempt to address some of the concerns which differentiate the iterated operator from an Anderson-type Hamiltonian. Namely, the necessity of choosing φ_k in a specific way based on the previous perturbation parameters, is confining.

The following theorems represent an exploration of how much control can be exerted over the absolutely continuous part of a spectral measure by a single perturbation, when no restriction is placed on the choice of the perturbation vector φ . A technical byproduct of losing this restriction is that the perturbation vector can not be assumed to be orthogonal to previous perturbations. The setup employed is representative of a spectral measure that would arise from the constructive iteration scheme after N steps.

Theorem 4.4.1. *Let $\mu \in M_+(\mathbb{R})$ be such that*

$$\mu = f\chi_{[-a,a]}dm + \sum_{n=1}^N \alpha_n \delta_{x_n},$$

where $f \in L^2[-a, a]$, $\|\mu\| = 1$ and $\sum_{n=1}^N \alpha_n = c$. Furthermore, let $\varphi \in L^2(\mu)$, φ be a unit vector and

$$\sum_{n=1}^N \alpha_n |\varphi(x_n)|^2 < \varepsilon.$$

Let the spectral measure of the self-adjoint operator

$$M_t + \lambda \langle \cdot, \varphi \rangle_{L^2(\mu)} \varphi \quad \text{on} \quad L^2(\mu),$$

with respect to φ , be denoted by μ_λ . Assume that I is a compact interval not including 0. Then for all $\lambda \in I$, there exists $k \in \mathbb{R}$ such that the spectral measure μ_λ satisfies

$$\|(\mu_\lambda)_{ac}\| \leq \|\mu_{ac}\| - k.$$

The theorem states that there is a minimum amount of absolutely continuous spectrum lost after a general perturbation

Proof. In order to simplify notation, all inner products are taken in $L^2(\mu)$ unless otherwise stated. Assume the hypotheses on f , μ and φ above. Decompose both φ and μ into two parts, one concerning the absolutely continuous spectrum on the interval $[-a, a]$, and the other concerning the N point masses. Hence, we define

$$\tilde{\varphi} = \varphi \chi_{[-a, a]}, \quad \varphi_p = \varphi - \tilde{\varphi} \quad \text{and} \quad \mu_{ac} = f \chi_{[-a, a]} dm, \quad \mu_p = \sum_{n=1}^N \alpha_n \delta_{x_n}.$$

The rank-one perturbation $\lambda \langle \cdot, \varphi \rangle \varphi$ can now be broken down in terms of $\tilde{\varphi}$ and φ_p so that the interaction between each part of the perturbation and the absolutely continuous spectrum can be estimated. The starting point for the strength of these interactions will be estimating the norm of the perturbation as follows:

$$\begin{aligned} \|\lambda \langle \cdot, \varphi \rangle \varphi\| &= |\lambda| \|\langle \cdot, (\tilde{\varphi} + \varphi_p) \rangle (\tilde{\varphi} + \varphi_p)\| \\ &\leq |\lambda| (\|\langle \cdot, \tilde{\varphi} \rangle \tilde{\varphi}\| + \|\langle \cdot, \tilde{\varphi} \rangle \varphi_p\| + \|\langle \cdot, \varphi_p \rangle \tilde{\varphi}\| + \|\langle \cdot, \varphi_p \rangle \varphi_p\|) \end{aligned} \quad (4.4.1)$$

The four terms in the inequality (4.4.1) will be discussed and evaluated separately. The first term, $|\lambda| \|\langle \cdot, \tilde{\varphi} \rangle \tilde{\varphi}\|$, involves only $\tilde{\varphi}$ so the perturbation of our

operator by this factor has no relevance to the point masses and is in fact orthogonal to μ_p . This scenario recreates a similar setting to our earlier results, where our perturbation vector was not concerned with the previous point masses due to orthogonality. The perturbation therefore has the effect of creating a single eigenvalue in the new spectral measure, determined solely by λ . In earlier results, the spectral measure was a constant on an interval thanks to our use of an auxiliary space and a choice of φ , so the mass of this eigenvalue was easy to compute. We have no such luxury here, as the choice of f has only the restriction that $f \in L^2[-a, a]$. Therefore, we solace ourselves with the ability to prove that there is a minimum for the mass of this eigenvalue, when λ is chosen from a compact interval not containing 0. Note however, that estimates for this value are attained in Proposition 4.4.2 below, with the corresponding loss of sharpness to the global estimate of k .

Let $h : \mathbb{R} \rightarrow \mathbb{R}$ be defined by $h(\lambda) = \mu_\lambda\{x_\lambda\}$, the mass of the created eigenvalue x_λ in the spectral representation, μ_λ of the perturbed operator $M_t + \lambda\langle \cdot, \varphi \rangle \varphi$. The explicit calculation of the location $x_\lambda \in \mathbb{R} \setminus [-a, a]$ and the strength $\mu_\lambda\{x_\lambda\}$ of the new eigenvalue is given by Aronszajn–Donoghue Theory. The process defining the function $h(\lambda)$ is thus given by two integrals:

$$\int_{-a}^a \frac{f(t)dt}{t - x_\lambda} = -\frac{1}{\lambda} \quad \text{and} \quad \mu_\lambda\{x_\lambda\} = G(x_\lambda) = \int_{-a}^a \frac{f(t)dt}{(t - x_\lambda)^2}. \quad (4.4.2)$$

As $f \in L^2[-a, a]$, both of these integrals are finite and yield continuous functions (actually C^1 by the definition of antiderivative), and the process of solving for x_λ after the first integral is as well. We conclude that $h(\lambda)$ is continuous itself, as the composition of continuous functions. Note that if $\tilde{\varphi}$ were acting on μ , not just μ_{ac} , then $h(\lambda)$ is not necessarily continuous as the point masses have to factor into the integral. Also, the domains of the Borel Transform and the integral operator $G(x_\lambda)$, in the usual sense, are equivalent to $L^2[-a, a]$ so this assumption was essential. Hence, if λ is chosen from a compact interval $I \subset \mathbb{R} \setminus \{0\}$ then $h(\lambda)$ must achieve a minimum value, referred to as d for the remainder of the paper, on I .

The second and fourth terms on the right hand side of the inequality (4.4.1) are easily dispatched with upon examination. Indeed, those two factors deal only with changes to the pure point spectrum, as the perturbations are in the “direction” of φ_p . Hence, the individual perturbations do not cause any change to the unperturbed absolutely continuous spectrum due to orthogonality of μ_p and μ_{ac}

The third term on the right hand side of the inequality (4.4.1), $|\lambda| \|\langle \cdot, \varphi_p \rangle \tilde{\varphi}\| \leq |\lambda| \|\varphi_p\| \|\tilde{\varphi}\|$, can be handled with our assumptions and above calculations, as $\|\varphi_p\|^2 < \varepsilon$. Indeed, φ_p only interacts with μ_p by definition, so

$$\|\varphi_p\|^2 = \langle \varphi_p, \varphi_p \rangle_{L^2(\mu_p)} = \sum_{n=1}^N \alpha_n |\varphi_p(x_n)|^2 = \sum_{n=1}^N \alpha_n |\varphi(x_n)|^2 \leq \varepsilon.$$

Similar reasoning yields that $\|\tilde{\varphi}\| = \sqrt{1 - \varepsilon}$. Hence, the estimate for this term will be $\|\langle \cdot, \varphi_p \rangle \tilde{\varphi}\| \leq \sqrt{\varepsilon} \sqrt{1 - \varepsilon}$.

Constructing the entire picture, we observe that the first term is how much the absolutely continuous spectrum is decreased by the creation of the new eigenvalue. The other term is correcting for what happens to the point masses, as there is no guarantee that some of the mass in μ_p doesn't reenter the interval $[-a, a]$ due to the effect of φ . Moreover, we know that the essential spectrum remains unchanged under our compact perturbation and that there is no total mass lost during the perturbation because the intertwining operator V_λ for the spectral theorem is unitary. We can now conclude

$$\|(\mu_\lambda)_{ac}\| \leq \|\mu_{ac}\| - [d - |\lambda| \sqrt{\varepsilon} \sqrt{1 - \varepsilon}].$$

The Theorem follows. □

In general, we cannot assume that $\|(\mu_\lambda)_{ac}\| \leq \|(\mu)_{ac}\|$. Therefore, it is imperative that $d - |\lambda| \sqrt{\varepsilon} \sqrt{1 - \varepsilon} > 0$ for the previous result to not be vacuous. Let $|\lambda|_{\max}$ denote the maximum value of $|\lambda|$ on I . Then the desired inequality is achieved when $d > |\lambda|_{\max} \sqrt{\varepsilon - \varepsilon^2}$. It is noteworthy that d was constructed to depend upon both λ

and the a.c. spectral mass, which directly relates to c and ε . More tangibly, we can directly estimate the value of d as follows.

Proposition 4.4.2. Let λ be chosen from I , a compact interval on the real line not including 0. Then

$$d \geq \frac{1 - c}{(a + |\lambda|_{\max}(1 - \varepsilon) + 1)^2},$$

where $|\lambda|_{\max}$ is the maximum value of $|\lambda|$ in I , and d , c and ε are as in the proof of Theorem 4.4.1.

Proof. Without loss of generality, we can assume that f is positive on the interval $[-a, a]$ and that $\lambda > 0$. This means that the eigenvalue created by the λ perturbation by $\tilde{\varphi}$ will be to the right of the interval, i.e. $|x_\lambda| > a$. For simplicity, we will also assume that we are working with the maximum value of λ in I instead of just any value for λ .

Recall the formulas in equation (4.4.2). Hence, to minimize $\mu_\lambda\{x_\lambda\}$, we minimize the kernel of the integral operator $G(x)$. This minimization occurs when f is represented by a delta mass at the endpoint $\{-a\}$ because then the eigenvalue will fall as close to a as possible. This delta mass is of strength $1 - c$ by necessity. Hence the integration $G(x_\lambda)$ becomes easy to compute and we find that

$$\mu_\lambda\{x_\lambda\} \geq \frac{1 - c}{(x_\lambda + 1)^2}.$$

To minimize this inequality we actually want to maximize the value of x_λ . The distance x_λ is placed from the endpoint a must be less than

$$\|\lambda\langle \cdot, \tilde{\varphi} \rangle \tilde{\varphi}\| = \lambda(1 - \varepsilon).$$

This means that $x_\lambda \leq a + \lambda(1 - \varepsilon)$. Finally, we can conclude that

$$\mu_\lambda\{x_\lambda\} \geq \frac{1 - c}{(x_\lambda + 1)^2} \geq \frac{1 - c}{(a + \lambda(1 - \varepsilon) + 1)^2}$$

as proposed. □

The following Corollary applies the approximations of the previous result to the specific case where f is a constant, as occurred during the iterative process.

Corollary 4.4.3. *Let $\mu \in M_+(\mathbb{R})$ be such that*

$$\mu = f\chi_{[-a,a]}dm + \sum_{n=1}^N \alpha_n \delta_{x_n},$$

where we define $f = w_N(t)$ such that $f \in L^1_{\text{loc}}$, $\|\mu\| = 1$ and $\sum_{n=1}^N \alpha_n = c$. Furthermore, let $\varphi \in L^2(\mu)$ such that $\varphi|_{[-a,a]} = 1/\sqrt{2w_N(t)}$, $\|\varphi\| = 1$ and $\sum_{n=1}^N \alpha_n |\varphi(x_n)|^2 < \varepsilon$. Assume that I is a compact interval not including 0. Then for all $\lambda \in I$, we have the following inequality

$$\|(\mu_\lambda)_{\text{ac}}\| \leq \|\mu_{\text{ac}}\| - \left[\frac{e^{1/\lambda\tau_N}}{\lambda^2\tau_N(e^{1/\lambda\tau_N} - 1)^2} - \frac{e^{1/\lambda\tau_N}\sqrt{\varepsilon}}{\lambda\tau_N(e^{1/\lambda\tau_N} - 1)^2} \right].$$

Proof. See the proof of the previous Theorem. In this case we have the assumption that

$$\tilde{\varphi}(t) = \frac{1}{\sqrt{2w_N(t)}}.$$

The notation $\tilde{\varphi}$ should not be confused with the image of φ under a unitary operator as in previous Sections. However, recall that $w_N(t)$ is simply representing a weight function and matches the notation developed in Section 4.3. In the case that λ is known, when Rademacher potentials are used for example, it is then possible to explicitly calculate the value of d . If a choice of λ has not been made, simply pick λ in the formula to be $|\lambda|_{\text{max}}$. \square

Similarly, we deduce how the singular part is effected by the perturbation at a single step.

Theorem 4.4.4. *Let $\mu \in M_+(\mathbb{R})$ be such that*

$$\mu = f\chi_{[-a,a]}dm + \sum_{n=1}^N \alpha_n \delta_{x_n},$$

where $f \in L^2(m)$, $\|\mu\| = 1$ and $\sum_{n=1}^N \alpha_n = c$. Furthermore, let $\varphi \in L^2(\mu)$, $\|\varphi\| = 1$ and

$$\sum_{n=1}^N \alpha_n |\varphi(x_n)|^2 < \varepsilon.$$

Let the spectral measure of the self-adjoint operator

$$M_t + \lambda \langle \cdot, \varphi \rangle_{L^2(\mu)} \varphi \quad \text{on} \quad L^2(\mu),$$

with respect to φ , be denoted by μ_λ . Assume that I is a compact interval not including 0. Then for all $\lambda \in I$, there exists $k \in \mathbb{R}$ such that the spectral measure μ_λ satisfies

$$\|(\mu_\lambda)_s\| \geq \|\mu_s\| + k.$$

Proof. We employ a similar strategy to the one used in Theorem 4.4.1. Namely, decompose the λ perturbation by decomposing φ into $\tilde{\varphi}$ and φ_p and estimate the inequality from (4.4.1):

$$\begin{aligned} \|\lambda \langle \cdot, \varphi \rangle \varphi\| &= |\lambda| \| \langle \cdot, (\tilde{\varphi} + \varphi_p) \rangle (\tilde{\varphi} + \varphi_p) \| \\ &\leq |\lambda| (\| \langle \cdot, \tilde{\varphi} \rangle \tilde{\varphi} \| + \| \langle \cdot, \tilde{\varphi} \rangle \varphi_p \| + \| \langle \cdot, \varphi_p \rangle \tilde{\varphi} \| + \| \langle \cdot, \varphi_p \rangle \varphi_p \|). \end{aligned}$$

However, this time we are only concerned with the first, second and fourth terms in the inequality, as they affect φ_p . The first term is responsible for creating an eigenvalue of strength at least d , as estimated above. The fourth term actually has no effect, as the essential spectrum of an operator does not change under a self-adjoint rank- perturbation. This means that the eigenvalues are shifted and masses are redistributed according to this term, but their total mass is the same because it cannot create s.c. or a.c. spectrum. Estimating the second term is analogous to the mixed term in Theorem 4.4.1 and yields an effect of $|\lambda| \sqrt{\varepsilon} \sqrt{1 - \varepsilon}$. Hence, the singular mass increases by a created eigenvalue and is adjusted for possible mass entering the absolutely continuous spectrum by a mixed term. Our conclusion thus follows its absolutely continuous counterpart and we set $k = d - |\lambda| \sqrt{\varepsilon} \sqrt{1 - \varepsilon}$ to yield the Theorem. \square

The same restrictions are relevant to applications of this theorem as to Theorem 4.4.1. In general, we cannot assume that $\|(\mu_\lambda)_s\| \geq \|\mu_s\|$, so for the result not to be vacuous we must have $d > |\lambda|_{\max} \sqrt{\varepsilon - \varepsilon^2}$ to ensure that $d - |\lambda| \sqrt{\varepsilon} \sqrt{1 - \varepsilon} > 0$. The symmetry of Theorems 4.4.1 and 4.4.4 adds further validation to the estimates.

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