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Spectra of Quantum Trees and Orthogonal Polynomials

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SPECTRA OF QUANTUM TREES AND ORTHOGONAL POLYNOMIALS

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Table of Contents

Abstract

We investigate the spectrum of regular quantum-graph trees, where the edges are endowed with a Schrödinger operator with self-adjoint Robin vertex conditions. It is known that, for large eigenvalues, the Robin spectrum approaches the Neumann spectrum. In this research, we compute the lower Robin spectrum. The spectrum can be obtained from the roots of a sequence of orthogonal polynomials involving two variables. As the length of the quantum tree increases, the spectrum approaches a band-gap structure. We find that the lowest band tends to minus infinity as the Robin parameter increases, whereas the rest of the bands remain positive. Unexpectedly, we find that two groups of isolated negative eigenvalues separate from the bottom of the lowest band. These eigenvalues are computed as they depend asymptotically on the Robin parameter. Our analysis invokes the interlacing property of orthogonal polynomials.

Chapter 1
Introduction

A quantum graph is a metric graph endowed with a Schrödinger operator on the edges. The Schrödinger operator is the minus second derivative plus a potential. People study quantum graphs for various reasons. They arise as reduced models in mathematics and physical sciences, especially in wave phenomena. Quantum graphs are related to partial differential equations. PDEs with extreme coefficients reduce to quantum graphs when the coefficients become localized along a graph-like set. At the other extreme, periodic quantum graphs act globally like PDEs, although they have the local structure ODEs coupled at endpoints.

Most problems in quantum graphs address how their spectral properties depend on the structure of the graph. We look at the spectrum of quantum tree graph, where the structure of the graph looks like an upside down tree as in Fig. 1.1. We call this tree graph Γ_n with n denoting the number of branching levels. The tree graph under investigation has the same degree $b+1$ at each vertex. Such a tree is called "regular", and b is called the branching number. In the appropriate context, the eigenvalues of Γ_n correspond to the frequencies, or energies, of the free standing waves in the structure. We investigate how the spectrum (characteristic energies) of such a graph depends on a certain self-adjoint vertex condition, known as the Robin condition. The "Robin parameter" is denoted by α in this dissertation.

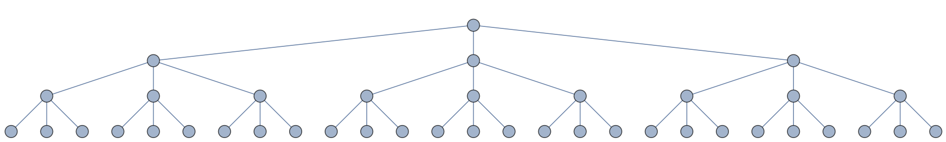

Figure 1.1. A quantum graph tree Γ_n with $n=3$ branching levels, each with branching number $b=3$.

It is known that Robin spectrum converges to the Neumann spectrum for high energy, and the high-energy asymptotics for the Neumann and Robin spectrum is known. This has been studied in depth by Carlson, Solomyak, and others [3, 4, 9, 11, 12, 13]. But at low energy, the spectrum of quantum trees varies greatly with the Robin parameter, and this dependence has not been investigated in depth up to now. More general results on the dependence of spectra of quantum graphs on the Robin vertex condition and interlacing properties have been proved by Schapotschnikow and Berkolaiko and Kuchment [10, 1]. The objective of this dissertation is to quantify in a very specific way the low-energy spectrum of quantum trees as it depends on the Robin parameter. The main tool in the analysis is the theory of orthogonal polynomials, especially the interlacing property of their roots and their asymptotics for large argument. One interesting discovery is the unexpected emergence of two rogue eigenvalues that split away from the lower end of the spectrum and tend to minus infinity as the Robin parameter becomes large and negative.

As a simple example for illustrating the dependence of spectrum on the Robin parameter, consider a Schrödinger operator on a single edge, identified with the interval $[0,1]$, with Robin boundary conditions. This is the rather very simple tree graph Γ_1 with $b = 1$. The eigenvalue problem for this operator is

$$\begin{aligned}&\Big(-\frac{d^2}{dx^2}+q(x)\Big)f(x)=\mu^2 f(x)\\&f'(0)=\alpha f(0) \text{ and } f'(1)=-\alpha f(1), \qquad \text{(Robin boundary condition)}\end{aligned}$$

in which $\lambda = \mu^2$ is the eigenvalue, or energy. When $q(x) = 0$, one computes that μ satisfies

$$\tan\mu = \frac{2\alpha\mu}{\mu^2-\alpha}.$$

This is the Neumann problem when $\alpha = 0$. We see that, when μ becomes large, the Robin spectrum approaches the Neumann spectrum ($\mu = k\pi$, where k is an integer). By contrast, the lower Robin spectrum deviates significantly from the Neumann spectrum. This observation holds for arbitrarily large trees, but as the tree becomes larger, it is no longer feasible to calculate the spectrum explicitly. It turns out that the Robin spectrum can be located accurately by identifying it with the roots of a sequence of orthogonal polynomials.

The eigenvalue problem for a Schrödinger operator A_n on a tree Γ_n with n levels is

$$\Big(-\frac{d^2}{dx^2} + q(x)\Big) f(x) = \lambda f(x) \tag{1.1}$$

$$\sum_{e\in\mathcal{E}(v)} f'_e(v) - \alpha f(v) = 0, \qquad \text{(Robin vertex condition)} \tag{1.2}$$

in which f is a function on Γ_n, $\mathcal{E}(v)$ is the set of edges adjacent to the vertex v, and the prime denotes the derivative out of the vertex into the edge. All of this will be made precise in the next section, including a careful definition of the domain of the Schrödinger operator. When the potential function $q(x)$ of a regular quantum tree is identical on all the edges, the tree is called "homogeneous". This thesis concerns the spectra of homogeneous quantum trees.

Briefly, the connection to orthogonal polynomials arises as follows. The problem (1.1, 1.2) is a system of linear ODEs on the edges coupled through the vertices via the Robin condition. The solution $f(x)$ is equivalently given by its values at the vertices, as long as λ is not a Dirichlet eigenvalue for any edge. The Robin condition amounts to a homogeneous linear system for these values. In the special case of completely symmetric eigenfunctions (constant across each level), the roots of its determinant $D_n(\lambda)$ are the eigenvalues of the quantum tree. This sequence satisfies a recursion relation, which, in the appropriate variable, precisely characterizes sequences of orthogonal polynomials. The location of the roots of D_n as a function of α is analyzed using interlacing properties for roots of orthogonal polynomials and the asymptotics of these polynomials for large arguments.

Numerical computations reveal an interesting behavior of the low-energy Robin spectrum. Particularly, as $\alpha \to -\infty$, two isolated groups of "rogue" eigenvalues separate from the lower end of the spectrum. Some numerical results are included in Figure 1.2.

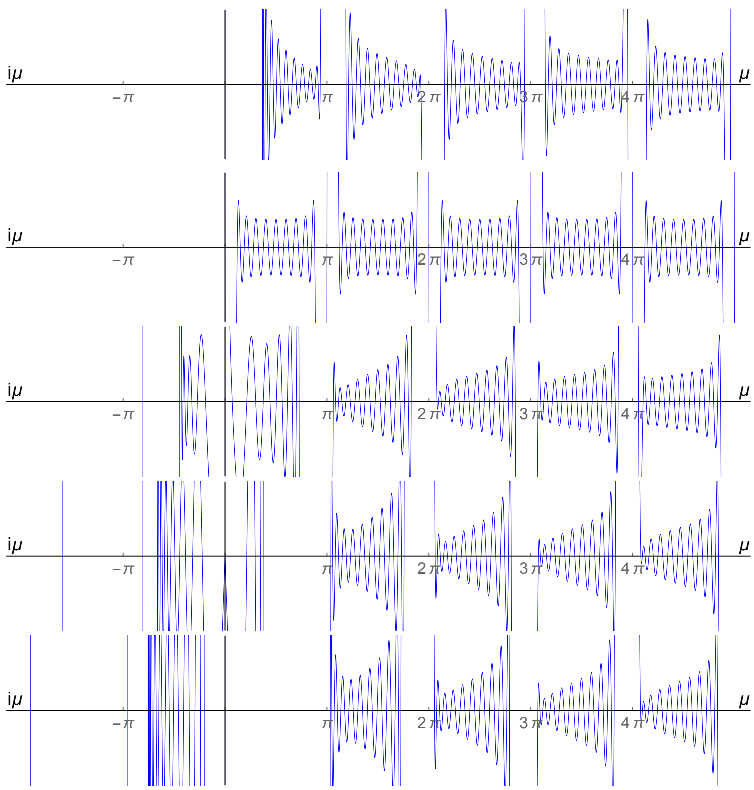

Figure 1.2. Graph of $D_{19}(\mu)$. The roots mark the square-root eigenvalues $\mu = \sqrt{\lambda}$ for the completely symmetric eigenfunctions of the quantum tree in Figure 1.1 with 19 levels. In each case, the branching number is 2, and, from top to bottom, the Robin constant α is 2, 0 (Neumann case), -2.5, -5, and -6.

Our goal is to find the asymptotic behavior of the low spectrum as the Robin parameter α tends to negatively large. To achieve this goal, this is what we are going to do in the following chapters of the thesis. In Chapter 2, we show how regular quantum trees are built starting with combinatorial graphs, then making them metric graphs by mapping each edge to the interval $[0,1]$, and finally putting a Schrödinger operator on the edges to make them quantum graphs. We carefully define the domain of the Schrödinger operator, which involves the Robin vertex condition. It has been proved in [2, Theorem 1.4.4] that on this domain, the Schrödinger operator is self-adjoint. Chapter 3 describes how the spectrum of a quantum tree Γ_n can be reduced by symmetry to the union of the spectra of $n+1$ linear graphs, with prescribed multiplicities.

In Chapter 4, we reduce the linear quantum trees to linear combinatorial graphs. With the assistance of the transfer matrix that involves two spectral functions $c(\lambda)$ and $s(\lambda)$ of the potential $q(x)$, we show that for a symmetric potential $q(x)$ and $s(\lambda) \neq 0$, that is, as long as λ is not a Dirichlet eigenvalue of the Schrödinger operator, the Robin vertex conditions amount to a homogeneous linear system with $(n+1) \times (n+1)$ matrix M_n. The roots of the determinant $D_n(\lambda)$ of the matrix $M_n(\lambda)$ give the eigenvalues of the linear quantum tree. We find that the functions $D_n(\lambda)$ satisfy a three-term recurrence relation in the variable n, which implies, by Favard's Theorem, that they are orthogonal polynomials in an appropriately chosen variable.

In Chapter 5, we analyze the spectrum of the quantum tree with theories from orthogonal polynomials. We define two sets of associated orthogonal polynomials $P_n(v)$ and $Q_n(v)$ that depend on the branching number b, and show that D_n is a linear combination of these with coefficients that depend on the Robin parameter and the spectral functions $c(\lambda)$ and $s(\lambda)$.

This connection to orthogonal polynomials allows us to analyze the spectrum of homogeneous quantum trees in a graphical way, as described at the beginning of Chapter 5. We think of the spectral functions $c(\lambda)$ and $s(\lambda)$ as defining a curve in (y,z)-space by $(y,z) = (c(\lambda), s(\lambda))$. This parametric curve depends on the potential $q(x)$. Meanwhile, the functions $D_n = D_n(y, z)$ become polynomials in two variables. The zero level sets of $D_n(y, z)$ in the yz-plane solely depend on the branching number b and the Robin parameter α. By looking at the intersections of the parametric curve and the zero level sets of D_n we obtain the precise location of the spectrum of regular homogeneous quantum trees. A useful feature of these two objects is that they separate the role of the potential $q(x)$ from the role of the Robin parameter α and the branching number b—the former determines the curve and the latter determine the level sets of D_n.

Chapter 2
Regular Quantum Trees

The regular quantum trees studied here are built with the following structure.

(1) Let an underlying tree graph Γ_n have vertex set $\mathcal{V}(\Gamma_n)$ and edge set $\mathcal{E}(\Gamma_n)$. It will always be depicted with the root vertex at the top with subsequent generations of vertices drawn along horizontal lines at different "levels". The ℓ-th generation of vertices will be called the ℓ-th level. Although the edges are technically undirected, the tree structure suggests a natural downward direction, and we shall refer to the top vertex as the origin vertex and the bottom ones as the terminal vertices. The vertices are arranged in levels 0 through n, and each vertex in level ℓ ($0 \leq \ell < n$) is connected by edges to b vertices in level $\ell+1$. The branching number b at any vertex is one less than the degree of the vertex (the number of edges incident to the vertex). This is illustrated in Fig. 1.1 for "branching number" $b = 3$. In combinatorial graph theory, edges are unordered pairs of vertices rather than geometric links.

(2) We then put additional structure on the combinatorial graph tree Γ_n that will make it a metric graph. The combinatorial graph Γ_n becomes a metric graph when each edge is parameterized by the normalized interval $[0, 1]$, oriented from level ℓ to level $\ell+1$, i.e. the original vertex is at $x = 0$ and the terminal vertex is at $x = 1$. The coordinate on edge e will be denoted by x_e or simply by x when appropriate. The set of points of a metric graph includes the vertices and all points along each edge. This allows the definition of standard function spaces on each edge e. We define the Lebesgue measure dx on the graph in the natural way with the x coordinate along the edges. With this measure, $H^s(e)$ is used to denote Sobolev space of functions on the segment e that have all their distributional derivatives

up to the order s belonging to $L^2(e)$. The space $L_2(\Gamma_n)$ on Γ_n consists of functions that are measurable and square integrable on each edge e and such that

$$\|f\|^2_{L_2(\Gamma_n)} := \sum_{e\in\mathcal{E}} \|f_e\|^2_{L_2(e)} < \infty \,, \tag{2.1}$$

in which f_e is the restriction of a function f on Γ_n to edge e. The Sobolev space $H^2(\Gamma_n)$ consists of all continuous functions on Γ_n that belong to $H^2(e)$ for each edge e and such that

$$\|f\|^2_{H_2(\Gamma_n)} := \sum_{e\in\mathcal{E}} \|f_e\|^2_{H_2(e)} = \sum_{e\in\mathcal{E}} \left(\|f_e\|^2_{L_2(e)} + \|f'_e\|^2_{L_2(e)} + \|f''_e\|^2_{L_2(e)}\right) < \infty \,. \tag{2.2}$$

(3) The metric tree Γ_n becomes a quantum tree when it is paired with a Schrödinger operator A_n. This is a differential operator whose form on each edge is

$$f(x) \;\mapsto\; -\frac{d^2 f}{dx^2}(x) + q(x)f(x), \tag{2.3}$$

A_n acts on functions $f = \{f_e\}_{e\in\mathcal{E}}$ defined on all of Γ_n and that satisfy a Robin condition at each vertex

$$\sum_{e\in\mathcal{E}(v)} f'_e(v) \;=\; \alpha_v\, f(v)\,, \tag{R}$$

in which f_e is the restriction of a function f on Γ_n to e, and $f'_e(v)$ is the derivative of f_e at the vertex v directed away from v. The vertex condition (R) is also known as a δ-type coupling or matching condition [6].

To define A_n precisely, first set

$$\begin{aligned} &H^2(\Gamma_n) \;= \\ &\left\{f = \{f_e\}_{e\in\mathcal{E}} : f \text{ is continuous; } f_e \in H^2(e)\, \forall e \in \mathcal{E}(\Gamma_n);\; f, f', f'' \in L^2(\Gamma_n)\right\}, \end{aligned} \tag{2.4}$$

in which the derivatives f' and f'' are taken on each edge with respect to the coordinates introduced above; and let $q \in L^2[0,1]$ be a real-valued potential function.

Then the domain of A_n and its action are given by

$$\mathcal{D}(A_n) = \left\{ f \in H^2(\Gamma_n) : f \text{ satisfies (R) } \forall\ v \in \mathcal{V}(\Gamma_n) \right\}, \tag{2.5}$$

$$(A_n f)(x) = -f''(x) + q(x) f(x)\,. \tag{2.6}$$

The Robin condition (R) makes sense because $f \in H^2(\Gamma_n)$ has well defined derivatives at the endpoints of each edge. On its domain $\mathcal{D}(A_n)$, A_n is a self-adjoint operator in $L^2(\Gamma_n)$. The self-adjointness follows from a general theorem [2, Theorem 1.4.4].

Chapter 3

Reduction of a Regular Tree to Linear Quantum Graphs

A regular homogeneous quantum graph (Γ_n, A_n) has a large group of symmetries. These symmetries allow one to reduce the operator to a direct sum of its action on invariant subspaces on which computation of the spectrum becomes tractable. This has been known since the work of Naimark and Solomyak [9, Theorem 7.2], and is described nicely in [13, §3]. This section describes how the spectrum of Γ_n can be reduced by symmetry to the union of the spectra of $n+1$ linear graphs, with prescribed multiplicities.

Let Γ_n^v denote the subtree of the graph Γ_n "below" the vertex v, that is, all vertices and edges that are descendants of v. If v is in level ℓ of Γ_n, then Γ_n^v is isomorphic, as a metric graph, to the tree $\Gamma_{n-\ell}$ of length $n-\ell$. Similarly, let Γ_n^e denote the subtree of Γ_n below the edge e and including e and both of its vertices. For any edge e connecting a vertex v at level ℓ to a vertex at the next level $\ell+1$, the subtree Γ_n^e is canonically isomorphic to a tree $\mathring{\Gamma}_{n-\ell}$ of length $n-\ell$, which is identical to $\Gamma_{n-\ell}$ except that the root vertex has only one edge incident to it.

The full symmetry group S_{Γ_n} of Γ_n is generated by applying to each subtree Γ_n^v all of the $b!$ permutations of the b trees Γ_n^e, where the edge e is emanating from v down to the next level. A permutation maps one of the trees Γ_n^e to another through the canonical identification of each with $\mathring{\Gamma}_{n-\ell}$. The operator A_n commutes with this symmetry group because all of the potentials q are the same on all edges and because the Robin constants α at all vertices are identical. For the purpose of decomposing A_n onto invariant subspaces, it is necessary to only consider a cyclic subgroup C_b of the permutations of the b edges e below v, since C_b is free and transitive on those edges. This cyclic symmetry group of Γ_n associated with v is denoted by C_b^v. Let C_{Γ_n} denote the subgroup of S_{Γ_n} that is generated by the groups C_b^v for each vertex $v \in \Gamma_n$.

The Fourier transform with respect to the symmetry group C_{Γ_n} produces the simplifying decomposition of (Γ_n, A_n). This decomposition is described in [9, Theorem 7.2], [12, §4], and [13, Theorem 3.2]. It proceeds as follows. Let $(\Gamma_n, A_n^{\rm sym})$ be the quantum tree equal to (Γ_n, A_n) restricted to the subdomain of $\mathcal{D}(A_n)$ that is invariant under the action of C_{Γ_n}, which means that $\mathcal{D}(A_n^{\rm sym})$ contains only those functions f in $\mathcal{D}(A_n)$ that are constant across all b^ℓ points (on edges or vertices) at any fixed level ℓ of Γ_n. Such functions f are called *completely symmetric*.

$$\begin{aligned} &\mathcal{D}(A_n^{\rm sym}) \;= \\ &\left\{ f \in H^2(\Gamma_n) : f \text{ satisfies (R) } \forall v \in \mathcal{V}(\Gamma_n) \text{ and } f \text{ is completely symmetric} \right\}. \end{aligned} \tag{3.1}$$

Also, let $(\Gamma_n, \mathring{A}_n^{\rm sym})$ be the completely symmetric quantum tree with the same differential operator on the edges but acting on the domain with the Dirichlet instead of Robin condition imposed at the root vertex v_0. Precisely,

$$\mathcal{D}(\mathring{A}_n^{\rm sym}) = \tag{3.2}$$

$$\Big\{ f \in H^2(\mathring{\Gamma}_n) : f(v_0) = 0 \text{ and } f \text{ satisfies (R) } \forall v \in \mathcal{V}(\Gamma_n) \backslash \{v_0\} \tag{3.3}$$

$$\text{and } f \text{ is completely symmetric}\}. \tag{3.4}$$

The main decomposition theorem says that

$$A_n \;\cong\; A_n^{\rm sym} \;\oplus\; \sum_{m=0}^{n} \left(\mathring{A}_m^{\rm sym}\right)^{(b-1)b^{n-m}}, \tag{3.5}$$

in which the power refers to the $(b-1)b^{n-m}$-fold direct sum of $\mathring{A}_m^{\rm sym}$ with itself.

The next step in the simplification of (Γ_n, A_n) is the reduction of $A_n^{\rm sym}$ and the associated operator $\mathring{A}_n^{\rm sym}$ to a Schrödinger operator on a linear metric tree graph

Λ_n with $n+1$ vertices and n edges, as depicted in Fig. 3.1. This process is described in [4] and in [12, §4, eqn. 6]. Essentially, since a function in $\mathcal{D}(A_n^{\text{sym}})$ or $\mathcal{D}(\mathring{A}_n^{\text{sym}})$ is invariant across any given level, it is determined by its value on a single edge of each level, so that all $b^{\ell+1}$ edges emanating down from vertices at level ℓ can be compressed into one. A function $f : \Lambda_n \to \mathbb{C}$ is denoted by the n-tuple $f = \{f_k\}_{k=1}^n$ of restrictions to the edges of Λ_n, in which each f_k is a function of the unit interval $[0, 1]$ that parameterizes the edge.

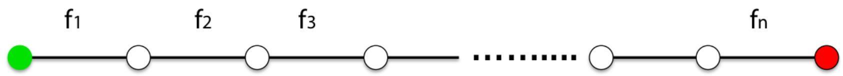

Figure 3.1. The totally symmetric eigenfunctions of the quantum tree in Fig. 1.1 are the eigenfunctions of this reduced graph with vertex conditions (R') depending on the branching numbers of the tree.

The Schrödinger operators B_n and $\mathring{B}_n$ on these linear quantum trees are self-adjoint with respect to a weighted L^2 inner product inherited from the original tree graph, when defined on the appropriate domain. For functions $f = \{f_k\}_{k=1}^n$ and $g = \{g_k\}_{k=1}^n$ on the linear metric graph, the inner product is

$$\langle f, g \rangle = \sum_{k=1}^{n} b^k \int_0^1 f_k(x)\, \bar{g}_k(x)\, dx\,. \tag{3.6}$$

The vertex condition (R) induces the following Robin condition for functions on Λ:

$$\begin{aligned} -f_i'(1) + bf_{i+1}'(0) - \alpha f_{i+1}(0) = 0 \quad (1 \le i \le n-1) \\ bf_1'(0) - \alpha f_1(0) = 0 \\ -f_n'(1) - \alpha f_n(1) = 0. \end{aligned} \tag{R'}$$

The domains of the Schrödinger operator B_n on Λ_n corresponding to A_n^{sym} is

$$\mathcal{D}(B_n) \;=\; \left\{ f = \{f_k\}_{k=1}^n \in H^2(\Lambda_n) : f \text{ satisfies (R')} \right\}. \tag{3.7}$$

The operator $\mathring{B}_n$ corresponding to $\mathring{A}_n^{\mathrm{sym}}$ is associated with boundary conditions that are modified to the Dirichlet condition at the root vertex,

$$\begin{aligned} -f_i'(1) + b f_{i+1}'(0) - \alpha f_{i+1}(0) &= 0 \quad 1 \leq i \leq n-1 \\ f_1(0) &= 0 \\ b f_n'(1) - \alpha f_n(1) &= 0. \end{aligned} \tag{R''}$$

The domain of this operator is

$$\mathcal{D}(\mathring{B}_n) \;=\; \left\{ f = \{f_k\}_{k=1}^n \in H^2(\Lambda_n) : f \text{ satisfies (R'')} \right\}. \tag{3.8}$$

The operators A_n^{sym} and B_n are unitarily similar to each other, as are the operators $\mathring{A}_n^{\mathrm{sym}}$ and $\mathring{B}_n$. The decomposition theorem now becomes

$$A_n \;\cong\; B_n \;\oplus\; \bigoplus_{m=0}^{n} \big(\mathring{B}_m\big)^{(b-1)b^{n-m}}. \tag{3.9}$$

The spectrum of A_n can now be computed by computing the spectrum of two types of linear quantum trees, B_n and $\mathring{B}_m$,

$$\sigma(A_n) \;=\; \sigma(B_n) \;\cup\; \bigcup_{m=0}^{n} \sigma(\mathring{B}_m). \tag{3.10}$$

Each of these spectra consists only of a discrete set of eigenvalues, and the eigenvalues of $\mathring{B}_m$ have multiplicity $(b-1)b^{n-m}$, provided all these $n+2$ spectral sets are mutually disjoint.

Chapter 4
Reduction to Linear Combinatorial Graphs

To reduce the linear quantum graphs to linear combinatorial graphs, we first consider the ordinary differential equation on a single edge. We parameterize the edge by the interval $[0,1]$. Consider two solutions $c(x,\lambda)$ and $s(x,\lambda)$ of the differential equation

$$-u''(x) + q(x)u(x) = \lambda u(x), \tag{4.1}$$

satisfying the initial conditions

$$\begin{aligned} c(0,\lambda) &= 1 \qquad & s(0,\lambda) &= 0 \\ c'(0,\lambda) &= 0 \qquad & s'(0,\lambda) &= 1, \end{aligned}$$

in which the prime denotes the derivative with respect to the first argument x. We can write

$$\begin{aligned} u(x) &= u(0)c(x,\lambda) + u'(0)s(x,\lambda) \\ u'(x) &= u(0)c'(x,\lambda) + u'(0)s'(x,\lambda), \end{aligned}$$

which in matrix form is

$$\begin{bmatrix} u(x) \\ u'(x) \end{bmatrix} = \begin{bmatrix} c(x,\lambda) & s(x,\lambda) \\ c'(x,\lambda) & s'(x,\lambda) \end{bmatrix} \begin{bmatrix} u(0) \\ u'(0) \end{bmatrix}.$$

The determinant of the matrix here is the Wronskian of the two solutions of (4.1), and is therefore constant in x. We see that it is equal to 1 by evaluating at $x = 0$.

We consider the outward derivatives at each vertex into the edge. Thus we will use $-u'(1)$ instead of $u'(1)$ in our calculation. The data $[u(1), -u'(1)]$ is related to data $[u(0), u'(0)]$ by

$$\begin{bmatrix} u(1) \\ -u'(1) \end{bmatrix} = \underbrace{\begin{bmatrix} c(1,\lambda) & s(1,\lambda) \\ -c'(1,\lambda) & -s'(1,\lambda) \end{bmatrix}}_{T(\lambda)} \begin{bmatrix} u(0) \\ u'(0) \end{bmatrix}. \tag{4.2}$$

The matrix here is called the transfer matrix $T(\lambda)$, and the determinant of $T(\lambda)$ is -1. We can thus write

$$\begin{bmatrix} c(1,\lambda) & s(1,\lambda) \\ -c'(1,\lambda) & -s'(1,\lambda) \end{bmatrix}^{-1} \begin{bmatrix} u(1) \\ u'(1) \end{bmatrix} = \begin{bmatrix} u(0) \\ -u'(0) \end{bmatrix}. \tag{4.3}$$

In the following lemma, we are going to show what happens if $q(x)$ is symmetric about the center of the edge. It is a significant simplification of the problem we are considering, because the result reduces the number of spectral functions in the transfer matrix $T(\lambda)$.

Lemma 1. *Suppose the potential $q(x)$ is symmetric about the center of the edge, meaning $q(1-x) = q(x)$. In this case, $c(1,\lambda) = s'(1,\lambda)$.*

Proof. Define the variable $y = 1-x$, which parameterizes the edge in the opposite direction. By defining

$$v(y) \ := \ u(1-y),$$

The differential equation (4.1) becomes

$$-v''(y) + q(1-y)v(y) = \lambda v(y).$$

Since q is symmetric, $v(y)$ satisfies the same differential equation as $u(x)$:

$$-v''(y) + q(y)v(y) = \lambda v(y).$$

Therefore, $v(y)$ also satisfies the transfer matrix equation 4.2, we can thus write

$$\begin{bmatrix} v(1) \\ -v'(1) \end{bmatrix} = \begin{bmatrix} c(1,\lambda) & s(1,\lambda) \\ -c'(1,\lambda) & -s'(1,\lambda) \end{bmatrix} \begin{bmatrix} v(0) \\ v'(0) \end{bmatrix}.$$

Now from
$$\begin{bmatrix} v(1) \\ -v'(1) \end{bmatrix} = \begin{bmatrix} u(0) \\ -u'(0) \end{bmatrix}, \text{ and } \begin{bmatrix} v(0) \\ v'(0) \end{bmatrix} = \begin{bmatrix} u(1) \\ u'(1) \end{bmatrix},$$
we obtain
$$\begin{bmatrix} u(0) \\ -u'(0) \end{bmatrix} = \begin{bmatrix} c(1,\lambda) & s(1,\lambda) \\ -c'(1,\lambda) & -s'(1,\lambda) \end{bmatrix} \begin{bmatrix} u(1) \\ u'(1) \end{bmatrix}. \tag{4.4}$$
Combining (4.3) and (4.4), we see that
$$\begin{bmatrix} c(1,\lambda) & s(1,\lambda) \\ -c'(1,\lambda) & -s'(1,\lambda) \end{bmatrix}^{-1} = \begin{bmatrix} c(1,\lambda) & s(1,\lambda) \\ -c'(1,\lambda) & -s'(1,\lambda) \end{bmatrix}.$$
We know that the determinant of the transfer matrix is -1, thus we have
$$\begin{bmatrix} s'(1,\lambda) & s(1,\lambda) \\ -c'(1,\lambda) & -c(1,\lambda) \end{bmatrix} = \begin{bmatrix} c(1,\lambda) & s(1,\lambda) \\ -c'(1,\lambda) & -s'(1,\lambda) \end{bmatrix}.$$
Hence under the symmetry assumption of $q(1-x) = q(x)$, we have $c(1,\lambda) = s'(1,\lambda)$. $\square$

For any symmetric potential q, define

$$c(\lambda) := c(1,\lambda) = s'(1,\lambda) \tag{4.5}$$
$$s(\lambda) := s(1,\lambda) \tag{4.6}$$
$$c'(\lambda) := c'(1,\lambda) \tag{4.7}$$
$$s'(\lambda) := s'(1,\lambda). \tag{4.8}$$

Lemma 2. *For symmetric $q(x)$ and $s(\lambda) \neq 0$, that is, as long as λ is not a Dirichlet eigenvalue of the Schrödinger operator $-d^2/dx^2 + q(x)$ on $[0,1]$, the derivatives of $u(x)$ at the endpoints are obtained from the values of $u(x)$ at the endpoints by*
$$\begin{bmatrix} u'(0) \\ -u'(1) \end{bmatrix} = \frac{1}{s(\lambda)} \begin{bmatrix} -c(\lambda) & 1 \\ 1 & -c(\lambda) \end{bmatrix} \begin{bmatrix} u(0) \\ u(1) \end{bmatrix}. \tag{4.9}$$

Proof. We can rewrite equation (4.2) with the transfer matrix $T(\lambda)$ as

$$\begin{bmatrix} u(1) \\ -u'(1) \end{bmatrix} = \begin{bmatrix} c(\lambda) & s(\lambda) \\ -c'(\lambda) & -s'(\lambda) \end{bmatrix} \begin{bmatrix} u(0) \\ u'(0) \end{bmatrix}$$

$\Longrightarrow$

$$\begin{aligned} u'(0) &= \frac{1}{s(\lambda)}(u(1) - c(\lambda)u(0)) \\ -u'(1) &= -c'(\lambda)u(0) - s'(\lambda)u'(0) \\ &= -c'(\lambda)u(0) - \frac{s'(\lambda)}{s(\lambda)}(u(1) - c(\lambda)u(0)) \\ &= \frac{1}{s(\lambda)}(-(c'(\lambda)s(\lambda) - s'(\lambda)c(\lambda))u(0) - s'(\lambda)u(1)) \\ &= \frac{1}{s(\lambda)}(u(0) - s'(\lambda)u(1)). \end{aligned}$$

Here we used the fact that

$$c'(\lambda)s(\lambda) - s'(\lambda)c(\lambda) = \det T(\lambda) = -1.$$

If $q(x)$ is centrally symmetric, then the relation $c(\lambda) = s'(\lambda)$ from the result of Lemma (1) yields

$$-u'(1) = \frac{1}{s(\lambda)}(u(0) - c(\lambda)u(1)).$$

Thus, when $s(\lambda) \neq 0$, the derivatives of $u(x)$ at the endpoints are obtained from the values of $u(x)$ by

$$\begin{aligned} u'(0) &= s(\lambda)^{-1}\left(u(1) - c(\lambda)u(0)\right) \\ -u'(1) &= s(\lambda)^{-1}\left(u(0) - c(\lambda)u(1)\right), \end{aligned}$$

which, in matrix form, is

$$\begin{bmatrix} u'(0) \\ -u'(1) \end{bmatrix} = \underbrace{\frac{1}{s(\lambda)} \begin{bmatrix} -c(\lambda) & 1 \\ 1 & -c(\lambda) \end{bmatrix}}_{G(\lambda)} \begin{bmatrix} u(0) \\ u(1) \end{bmatrix}. \tag{4.10}$$

Here $G(\lambda)$ is exactly the Dirichlet-to-Neumann map. $\square$

Given that the functions $u_k(x)$ on the edges of the linear quantum graph satisfy the eigenvalue equation $-u_k'' + q(x)u_k = \lambda u_k$, Lemma 2 implies that the Robin condition (R") at all vertices of the linear graph can be written solely in terms of the values of the functions at the vertices—that is, if $s(\lambda) \neq 0$. Those values of λ for which $s(\lambda) = 0$ are exactly the Dirichlet eigenvalues of $-d^2/dx^2 + q(x)$ on $[0, 1]$. These values will be treated at the end of this chapter in Proposition 4.

Continuity of the function $\{u_k(x_e)\}_{k=0}^n$ on the graph allows one to define

$$\begin{aligned} u_0 &:= u_1(0) \\ u_k &:= u_{k+1}(0) = u_k(1) \\ u_n &:= u_n(1), \end{aligned}$$

and from Lemma 2, we can deduce the values of derivatives of the functions u_k at the vertices in terms of the function values at the vertices

$$\begin{aligned} u_{k+1}'(0) &= \frac{1}{s}(u_{k+1} - cu_k) \\ -u_{k+1}'(1) &= \frac{1}{s}(u_k - cu_{k+1}) \end{aligned} \tag{4.11}$$

where $s = s(\lambda)$ and $c = c(\lambda)$.

For a quantum tree with n levels, the Robin vertex conditions

$$bu_1'(0) = \alpha u_1(0)$$

$$-u_k'(1) + bu_{k+1}'(0) = \alpha u_k(1) \quad (0 < k < n)$$

$$-u_n'(1) = \alpha u_n(1),$$

together with equations (4.11) generate these equations

$$b\frac{1}{s}(u_1 - cu_0) = \alpha u_0$$

$$\frac{1}{s}(u_{k-1} - cu_k) + b\frac{1}{s}(u_{k+1} - cu_k) = \alpha u_k \quad (0 < k < n)$$

$$\frac{1}{s}(u_{n-1} - cu_n) = \alpha u_n.$$

When $s \neq 0$, these equations can be written as

$$-(cb + s\alpha)u_0 + bu_1 = 0$$

$$u_{k-1} - (c(b+1) + s\alpha)u_k + bu_{k+1} = 0 \quad (0 < k < n)$$

$$u_{n-1} - (c + s\alpha)u_n = 0.$$

This is a homogeneous system for $\{u_k\}_{k=0}^{n}$ with $(n+1)\times(n+1)$ matrix of coefficients

$$M_n = \begin{bmatrix} cb + s\alpha & -b & 0 & 0 & 0 & 0 \\ -1 & c(b+1) + s\alpha & -b & 0 & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \vdots & 0 & \ddots & c(b+1) + s\alpha & -b \\ 0 & \vdots & 0 & 0 & -1 & c + s\alpha \end{bmatrix}.$$

Define the determinants

$$\begin{aligned} D_n &= \det M_n \quad (n \geq 1) \\ D_0 &= s\alpha \\ D_{-1} &= 1 - c^2\,. \end{aligned} \tag{4.12}$$

For the case of the Dirichlet condition at the root vertex (but retaining Robin conditions at the other vertices), just the first row of the matrix of coefficients differs from the Robin case. The new matrix is

$$\mathring{M}_n = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & c(b+1) + s\alpha & -b & 0 & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \vdots & 0 & \ddots & c(b+1) + s\alpha & -b \\ 0 & \vdots & 0 & 0 & -1 & c + s\alpha \end{bmatrix}.$$

Define the determinants

$$\begin{aligned} \mathring{D}_n &= \det \mathring{M}_n \quad (n \geq 1) \\ \mathring{D}_0 &= 1 \\ \mathring{D}_{-1} &= c\,. \end{aligned} \tag{4.13}$$

Theorem 3. *The quantities D_n and $\mathring{D}_n$ satisfy the same second-order recurrence relation*

$$D_n \;=\; [c(b+1)+s\alpha]\, D_{n-1} - b\, D_{n-2} \qquad (n \geq 1) \tag{4.14}$$

$$\mathring{D}_n \;=\; [c(b+1)+s\alpha]\, \mathring{D}_{n-1} - b\, \mathring{D}_{n-2} \qquad (n \geq 1). \tag{4.15}$$

Proof. Define N_n to be the $(n+1)\times(n+1)$ matrix whose entries are identical to those of M_n except that the $(n+1, n+1)$ (lower right) entry is $c(b+1)+s\alpha$ in place of $c+s\alpha$. Define the determinants

$$E_n = \det N_n \quad (n \geq 0).$$

Then E_n satisfies the recursion relation

$$\begin{aligned} E_n \;&=\; [c(b+1)+s\alpha]\, E_{n-1} - b\, E_{n-2} \\ E_{-1} &= 1 \\ E_{-2} &= \frac{c}{b}\,. \end{aligned} \tag{4.16}$$

The initial conditions come from knowing that

$$\begin{aligned} E_0 &= cb + s\alpha \\ E_1 &= [c(b+1)+s\alpha](cb+s\alpha) - b. \end{aligned}$$

One thus computes that

$$D_n = E_n - cb\, E_{n-1} \qquad (n \geq -1). \tag{4.17}$$

We shift the index of the recursion relation of E_n by one yields this set of equations

$$\begin{aligned} E_n &= [c(b+1)+s\alpha]E_{n-1} - bE_{n-2} \qquad (n \geq 0) \\ E_{n-1} &= [c(b+1)+s\alpha]E_{n-2} - bE_{n-3} \qquad (n \geq 1). \end{aligned} \tag{4.18}$$

The first of these equations minus cb times the second one produces the desired recurrence relation for the $\{D_n\}$.

The recurrence for the $\{\mathring{D}_n\}$ is established similarly. Define the matrices $\mathring{N}_n$ by replacing the $(n+1, n+1)$ (lower right) entry of $\mathring{M}_n$ by $c(b+1) + s\alpha$, and define

$$\begin{aligned} \mathring{E}_n &= \det \mathring{N}_n \quad n \geq 0 \\ \mathring{E}_{-1} &= 0 \\ \mathring{E}_{-2} &= -\frac{1}{b} \,. \end{aligned} \tag{4.19}$$

Again, one computes the relations $\mathring{D}_n = \mathring{E}_n - cb\,\mathring{E}_{n-1}$ $(n \geq -1)$ and $\mathring{E}_n = [c(b+1) + s\alpha]\mathring{E}_{n-1} - b\mathring{E}_{n-2}$ $(n \geq 0)$ and thence the desired recurrence for $\{\mathring{D}_n\}$. □

The rescaled quantities $\tilde{D}_n = b^{\frac{n}{2}} D_n$ are more suitable for viewing the graphs of the functions. They satisfy the recursion

$$\begin{aligned} \tilde{D}_n &= b^{-\frac{1}{2}}[c(b+1) + s\alpha]\tilde{D}_{n-1} - \tilde{D}_{n-2} \\ \tilde{D}_0 &= s\alpha \\ \tilde{D}_{-1} &= b^{\frac{1}{2}}(1 - c^2). \end{aligned}$$

Similarly, define $\tilde{\mathring{D}}_n = b^{\frac{n}{2}} \mathring{D}_n$, and the recursion relation for $\tilde{\mathring{D}}_n$ is

$$\begin{aligned} \tilde{\mathring{D}}_n &= b^{-\frac{1}{2}}[c(b+1) + s\alpha]\tilde{\mathring{D}}_{n-1} - \tilde{\mathring{D}}_{n-2} \\ \tilde{\mathring{D}}_0 &= 1 \\ \tilde{\mathring{D}}_{-1} &= b^{\frac{1}{2}} c \,. \end{aligned}$$

We now treat those values of λ for which $s(\lambda) = 0$. It turns out that typically, these are not eigenvalues of (Γ, A)—but they are for $\alpha = 0$ and $q(x) = 0$.

Proposition 4. *Suppose that $q(x) = q(1-x)$ and that $s(\lambda) = 0$.*

(i) For all integers $m \geq 1$, λ is not an eigenvalue of $(\Lambda_m, \mathring{B}_m)$.

(ii) If $\alpha = 0$ and $c'(\lambda) = 0$, then for all positive integers n, λ is an eigenvalue of (Λ_n, B_n).

(iii) If $\alpha \neq 0$ or $c'(\lambda) \neq 0$, then for sufficiently large integers n, λ is not an eigenvalue of (Λ_n, B_n).

Proof. When $s(\lambda) = 0$ and $q(x) = q(1-x)$, one has

$$\begin{bmatrix} c(\lambda) & s(\lambda) \\ c'(\lambda) & s'(\lambda) \end{bmatrix} = \begin{bmatrix} (-1)^{n+1} & 0 \\ c'(\lambda) & (-1)^{n+1} \end{bmatrix}.$$

The Robin conditions (R') and (R") imply for vertices $\ell = 1 \dots n$ of Λ,

$$\begin{bmatrix} u_{\ell+1}(0) \\ u'_{\ell+1}(0) \end{bmatrix} = \begin{bmatrix} \pm 1 & 0 \\ b^{-1}(c'(\lambda) \mp \alpha) & \pm b^{-1} \end{bmatrix} \begin{bmatrix} u_\ell(0) \\ u'_\ell(0) \end{bmatrix}, \tag{4.20}$$

in which we make the definitions $u'_{n+1}(0) := 0$ and $u_{n+1}(0) := u_n(1)$.

For $(\Lambda, \mathring{B}_n)$, $u_1(0) = 0$, so $u_n(1) = u_{n+1}(0) = 0$, and $0 = u'_{n+1}(0) = (\pm 1)^n b^{-n} u'_1(0)$. Thus $u'_1(0) = 0$ and $u_1(x)$ vanishes identically. Inductively using the Robin condition on all the vertices, one obtains that $u_\ell(x) = 0$ identically for all ℓ, and so λ is not an eigenvalue of $\mathring{B}_n$.

For (Λ, B_n), the Robin condition at the root vertex 0 implies that

$$[u_0(0), u'_0(0)] \propto [b, -\alpha].$$

To satisfy the Robin condition at all vertices, condition (4.20) must hold for $\ell = 0 \dots n$, together with the stipulation that $u'_{n+1}(0) = 0$. Denote $v_\ell = u'_\ell(0)$. In the $+1$ case, the relation (4.20) implies the nonhomogeneous recursion

$$\begin{aligned} v_0 &= -\alpha \\ v_{\ell+1} - v_\ell &= -(1 - b^{-1}) \left(v_\ell - \frac{c'(\lambda) - \alpha}{1 - b^{-1}} \right), \end{aligned}$$

and in the -1 case, one obtains

$$\begin{aligned}
v_0 &= -\alpha \\
v_1 &= c'(\lambda) + (1 + b^{-1})\alpha \\
v_{\ell+2} - v_\ell &= -(1 - b^{-2})\left(v_\ell \,+\, (-1)^\ell\,\frac{(1 + b^{-1})(c'(\lambda) + \alpha)}{1 - b^{-2}}\right).
\end{aligned}$$

If α and $c'(\lambda)$ both vanish, then $v_\ell = 0$ for all ℓ; in particular, for $\ell = n + 1$, one obtains $v_{n+1} = 0$ which is exactly the requirement of the Robin condition (4.20) for $\ell = n$ with the stipulation that $u'_{n+1}(0) = 0$. Thus λ is an eigenvalue of B_n for each n.

The sequence v_n converges to $(c'(\lambda) - \alpha)/(1 - b^{-1})$ in the $+1$ case and to the sequence $(-1)^\ell(1 + b^{-1})(c'(\lambda) + \alpha)/(1 - b^{-2})$ in the -1 case. Thus, if $\alpha \neq 0$ or $c'(\lambda) \neq 0$, one has $v_\ell \neq 0$ for ℓ sufficiently large so that the stipulation $u'_{n+1}(0) = 0$ cannot be satisfied for sufficiently large n. This means that λ is not an eigenvalue of B_n for sufficiently large n. $\square$

Chapter 5
Analysis of Spectrum via Orthogonal Polynomials

So far, c and s are tied to each other through λ. But through the recursion relations, D_n can be viewed as a function of two variables c and s. By calling these variables y and z, we can think of $c(\lambda)$ and $s(\lambda)$ as defining a curve in (y, z)-space by $(y, z) = (c(\lambda), s(\lambda))$. When replacing the spectral functions $c(\lambda)$ and $s(\lambda)$ in D_n and $\mathring{D}_n$ by independent variables y and z, the functions $D_n = D_n(y, z)$ and $\mathring{D}_n = \mathring{D}_n(y, z)$ become polynomials in two variables. An energy λ, is an eigenvalue of the associated linear quantum graph with n edges whenever

$$D_n\big(c(\lambda), s(\lambda)\big) = 0. \tag{5.1}$$

This point of view has the advantage that the spectrum is represented geometrically by the intersection points of two objects in the yz-plane that separate the role of the parameters α and b from the role of the potential $q(x)$. These objects are

1. The zero sets $D_n(y, z) = 0$ and $\mathring{D}_n(y, z) = 0$ are determined by the Robin parameter α and the splitting degree b of the original quantum tree. Both appear in the recurrence relation given by Theorem 3, and α appears in the initial condition for D_n (4.12).

2. The curve in the yz-plane parameterized by $y = c(\lambda)$ and $z = s(\lambda)$ for real λ is determined solely by the potential $q(x)$.

The superposition of these two objects is shown in Figure 5.1.

5.1 The zero sets of $D_n(y, z)$ and $\mathring{D}_n(y, z)$

Since the recurrence relation satisfied by both D_n and $\mathring{D}_n$ involves y and z only through the composite variable

$$v = (b + 1)y + \alpha z, \tag{5.2}$$

it is convenient to define two sequences of polynomials in v,

$$P_n(v) = v\,P_{n-1}(v) - b\,P_{n-2}(v), \quad P_{-1} = 0, \quad P_0 = 1, \tag{5.3}$$

$$Q_n(v) = v\,Q_{n-1}(v) - b\,Q_{n-2}(v), \quad Q_{-1} = 1, \quad Q_0 = 0. \tag{5.4}$$

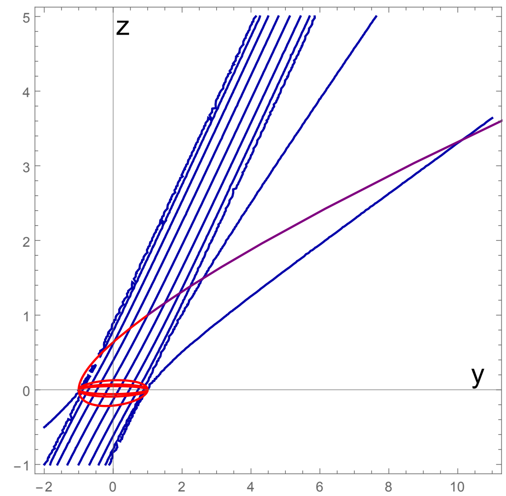

Figure 5.1. The blue curves form the zero-set of the polynomial $D_9(x, z)$. Their intersection with the spiral curve ($x = \cos\mu$, $z = \mu^{-1}\sin\mu$) for $q(x) = 0$ determine the eigenvalues $\lambda = \mu^2$ of A_n.

Notice that both $P_n(v)$ and $Q_n(v)$ satisfy a three-term recurrence relation. Moreover, these recurrence relations have constant coefficients independent of n. We know that orthogonal polynomials have the property of three-term recurrence relation. Favard's Theorem [5, Chapter I, Theorem 4.4] tells us that conversely, a sequence of polynomials with three-term recurrence relation (subject to certain conditions) is a sequence of orthogonal polynomials with respect to a moment functional $\mathcal{L}$, which induces an inner product with respect to a certain measure. This means that, for a function $p(x)$, $\mathcal{L}(p(x)) = \int p(x)d\psi(x)$ for some increasing function ψ of bounded variation. The induced inner product is

$$< p_1(x), p_2(x) >= \mathcal{L}(p_1(x)p_2(x)) = \int p_1(x)p_2(x)d\psi(x).$$

The moments of $d\psi$ are

$$\mu_n = \int x^n d\psi(x).$$

Moreover, Favard's Theorem [5, Chapter I, Theorem 4.4] also says that for our orthogonal polynomials $P_n(v)$,

$$\mu_0 = \mathcal{L}[1] = b\ . \tag{5.5}$$

This is also true for the orthogonal polynomial $Q_n(v)$, because it has the same recurrence relation as $P_n(v)$. In the next proposition, we are going to see how exactly $P_n(v)$ and $Q_n(v)$ are related to each other.

Proposition 5. *(i) Both the sequences $\{P_n(v)\}_{n=0}^{\infty}$ and $\{Q_n(v)\}_{n=0}^{\infty}$ are orthogonal polynomials in v.*

(ii) They are related by $-bP_n(v) = Q_{n+1}(v)$.

Proof. The first part is already proved by the discussion above this proposition. We now prove the second part.

Notice that $P_n(v)$ and $Q_n(v)$ have constant coefficients in the recurrence relations. Since $Q_{-1}(v) = 1$, $Q_0(v) = 0$, by the recurrence relation in (5.3), we obtain $Q_1(v) = -b$. Let $P_n^{(1)}(v) = (-b)^{-1}Q_{n+1}(v)$. Then $P_n^{(1)}(v)$ satisfies the recurrence relation

$$P_n^{(1)}(v) = vP_{n-1}^{(1)}(v) - bP_{n-2}^{(1)}(v), \quad P_{-1}^{(1)}(v) = 0, \quad P_0^{(1)}(v) = 1.$$

Thus we see that $P_n^{(1)}(v) = P_n(v)$. We hence obtain that $P_n(v) = (-b)^{-1}Q_{n+1}(v)$. The relation $-bP_n(v) = Q_{n+1}(v)$ is thus proved.

□

We see that $P_n(v)$ is an n-th degree polynomial. We denote the roots of $P_n(v)$ as

$$\{v \in \mathbb{R} : P_n(v) = 0\} = \{v_{n1}, \ldots v_{nn}\}\ . \tag{5.6}$$

Similarly, Q_n has degree $n-1$. We use the following notation for the roots of $Q_n(v)$:

$$\{v \in \mathbb{R} : Q_n(v) = 0\} = \{w_{n1}, \dots w_{n,n-1}\} . \tag{5.7}$$

In terms of the two sequences of orthogonal polynomials $P_n(v)$ and $Q_n(v)$, one has

$$\left.\begin{aligned} D_n(y,z) &= D_n^\alpha(y,z) = \alpha z\, P_n(v) + (1-y^2)\, Q_n(v)\,, \\ \mathring{D}_n(y,z) &= \mathring{D}_n^\alpha(y,z) = P_n(v) + y\, Q_n(v)\,, \end{aligned}\right\} \quad \text{with } \ v = (b+1)y + \alpha z. \tag{5.8}$$

Since $P_n(v)$ is an nth degree orthogonal polyomial corresponding to the moment functional $\mathcal{L}$, we would like to have a discussion of $\mathcal{L}$ here. Suppose that $\mathcal{L}$ is positive-definite with moment sequence $\{\mu_n\}_{n=0}^{\infty}$. The Gaussian quadrature formula [5, Chapter I, Theorem 6.1] tells us that for $j \leqslant 2n-1$, there are positive numbers $A_{n1}, \dots, A_{nn}$ such that

$$\int v^j d\psi(v) = \mathcal{L}[v^j] = \mu_j = \sum_{i=1}^{n} A_{ni} v_{ni}^j, \quad j = 0, 1, \dots, 2n-1, \tag{5.9}$$

where $v_{n1} < v_{n2} < \cdots < v_{nn}$ are the roots of $P_n(v)$. We define ψ_n by

$$\psi_n(v) = \begin{cases} 0 & \text{if } v < v_{n1} \\ A_{n1} + A_{n2} + \cdots + A_{np} & \text{if } v_{np} \leq \ \ v < v_{n,p+1} \quad (1 \leq p < n) \\ \mu_0 & \text{if } v \geq v_{nn} \end{cases}$$

Thus, $\psi_n(v)$ is a bounded, right continuous, non-decreasing step function whose jump set is the finite set $\{v_{n1}, \dots, v_{nn}\}$, and whose jump at v_{ni} is $A_{ni} > 0$. With this definition, we can write the sum as a Stieljes integral

$$\int_{-\infty}^{\infty} f(v) d\psi_n(v) = \sum_{i=1}^{n} A_{ni} f(v_{ni}).$$

Hence

$$\int_{-\infty}^{\infty} v^j d\psi_n(v) = \sum_{i=1}^{n} A_{ni} v_{ni}^j = \mu_j, \quad j = 0, 1, \dots, 2n-1.$$

Equation (5.9) means that

$$\int v^k d\psi_n(v) = \int v^k d\psi(v), \quad \text{for } k \le 2n-1.$$

Thus $d\psi_n$ approximates $d\psi$ as a measure in the sense that $d\psi_n$ produces integrals of polynomials of degree $k \le 2n-1$ exactly. Later on, we will make use of all moments of $d\psi_n$, and so we define

$$\mu_j^{(n)} = \int v^j d\psi_n(v), \text{ for } j = 1, 2, \ldots, \text{ and } n = 1, 2, \ldots.$$

Equation (5.9) now takes the simple form

$$\mu_j^{(n)} = \mu_j, \quad \text{for } j \le 2n-1.$$

In the proposition coming up, we will see that $P_n(v)$ and $Q_n(v)$ are either even or odd polynomials depending on n. Therefore, their roots are symmetric about the origin. Thus $\int v^j d\psi_n(v) = 0$ when j is odd, which means $\mu_j^{(n)} = 0$ when j is odd. Similarly, $\int v^j d\psi(v) = 0$ when j is odd also. We will use this fact to simplify our calculations later on.

Now let's first explore some properties of these orthogonal polynomials $P_n(v)$ and $Q_n(v)$.

Proposition 6. *(i) P_n and Q_n are even or odd polynomials in v. For $n \ge 1$, $P_n(v)$ is the polynomial part of*

$$v^n - (n-1)b\,v^{n-2} + \frac{(n-3)(n-2)}{2}b^2 v^{n-4} - \frac{(n-5)(n-4)(n-3)}{6}b^3 v^{n-6} + \ldots,$$

and $Q_n(v)$ is the polynomial part of

$$-b\,v^{n-1} + (n-2)b^2\,v^{n-3} - \frac{(n-4)(n-3)}{2}b^3 v^{n-5} + \frac{(n-6)(n-5)(n-4)}{6}b^4 v^{n-7} + \ldots,$$

in which the ellipses indicate lower-degree monomials.

(ii) For $n \geq -1$,

$$\begin{aligned} D_n(-y,-z) &= (-1)^{n+1} D_n(y,z) \\ \mathring{D}_n(-y,-z) &= (-1)^n \mathring{D}_n(y,z) \\ D_n^{-\alpha}(-y,z) &= (-1)^{n+1} D_n^{\alpha}(y,z) \\ \mathring{D}_n^{-\alpha}(-y,z) &= (-1)^n \mathring{D}_n^{\alpha}(y,z)\,. \end{aligned} \tag{5.10}$$

(iii) The roots of P_n and Q_n interlace each other, as do the roots of P_n and P_{n+1} and the roots of Q_n and Q_{n+1}.

(iv) The roots of P_n and the roots of Q_n lie between $-(b+1)$ and $(b+1)$.

Proof. (i) From the recursion relation and initial conditions of

$$P_n(v) = v\,P_{n-1}(v) - b\,P_{n-2}(v), \quad P_0 = 1, \quad P_{-1} = 0,$$

we can write out the first few terms of P_n and obtain the general form by induction:

$$\begin{aligned} P_1 &= v \\ P_2 &= vP_1 - bP_0 = v^2 - b \\ P_3 &= vP_2 - bP_1 = v^3 - 2bv \\ P_4 &= vP_3 - bP_2 = v^4 - 3bv^2 + b^2 \\ &\vdots \end{aligned}$$

$$P_n(v) = v^n - (n-1)b\,v^{n-2} + \frac{(n-3)(n-2)}{2}b^2v^{n-4} - \frac{(n-5)(n-4)(n-3)}{6}b^3v^{n-6} + \ldots$$

Therefore, when n is even, P_n is even, when n is odd, P_n is odd.

For the general form of Q_n, we again obtain the general form by induction from the recursion relation and the initial conditions.

$$Q_n(v) = v\,Q_{n-1}(v) - b\,Q_{n-2}(v), \quad Q_0 = 0, \quad Q_{-1} = 1$$

$$\begin{aligned}
\Longrightarrow \quad & Q_1 = -b \\
& Q_2 = -bv \\
& Q_3 = -bv^2 + b^2 \\
& Q_4 = -bv^3 + 2b^2 v \\
& \quad \vdots
\end{aligned}$$

$$Q_n(v) = -b\,v^{n-1} + (n-2)b^2\,v^{n-3} - \frac{(n-4)(n-3)}{2} b^3 v^{n-5} + \\ + \frac{(n-6)(n-5)(n-4)}{6} b^4 v^{n-7} + \dots$$

Therefore, when n is even, Q_n is odd, and when n is odd, Q_n is even.

(ii) Notice that

$$(y, z) \mapsto (-y, -z) \quad \Rightarrow \quad v \mapsto -v$$

$$(y, \alpha) \mapsto (-y, -\alpha) \quad \Rightarrow \quad v \mapsto -v$$

And we have

$$\begin{aligned}
D_n(y, z) = D_n^\alpha(y, z) &= \alpha z\,P_n(v) + (1 - y^2)\,Q_n(v) \\
\mathring{D}_n(y, z) = \mathring{D}_n^\alpha(y, z) &= P_n(v) + y\,Q_n(v)\,.
\end{aligned}$$

Thus we can derive

$$\begin{aligned}
D_n(-y, -z) &= -\alpha z\,P_n(-v) + (1 - y^2)\,Q_n(-v) \\
(\text{when } n \text{ is even}) &= -\alpha z\,P_n(v) - (1 - y^2)\,Q_n(v) = -D_n(y, z) \\
(\text{when } n \text{ is odd}) &= \alpha z\,P_n(v) + (1 - y^2)\,Q_n(v) = D_n(y, z).
\end{aligned}$$

Therefore,

$$D_n(-y, -z) = (-1)^{n+1} D_n(y, z).$$

Similarly,

$$\mathring{D}_n(-y,-z) = P_n(-v) - y\,Q_n(-v)$$
$$(\text{when } n \text{ is even}) = P_n(v) + y\,Q_n(v) = \mathring{D}_n(y,z)$$
$$(\text{when } n \text{ is odd}) = -P_n(v) - y\,Q_n(v) = -\mathring{D}_n(y,z).$$

Thus we obtain

$$\mathring{D}_n(-y,-z) = (-1)^n \mathring{D}_n(y,z).$$

The last two equations in this part of the proposition are shown with similar arguments as above.

$$D_n^{-\alpha}(-y,z) = -\alpha z\,P_n(-v) + (1-y^2)\,Q_n(-v)$$
$$(\text{when } n \text{ is even}) = -\alpha z\,P_n(v) - (1-y^2)\,Q_n(v) = -D_n^{\alpha}(y,z)$$
$$(\text{when } n \text{ is odd}) = \alpha z\,P_n(v) + (1-y^2)\,Q_n(v) = D_n^{\alpha}(y,z).$$

Therefore,

$$D_n^{-\alpha}(-y,z) = (-1)^{n+1} D_n^{\alpha}(y,z).$$

Similarly,

$$\mathring{D}_n^{-\alpha}(-y,z) = P_n(-v) - y\,Q_n(-v)$$
$$(\text{when } n \text{ is even}) = P_n(v) + y\,Q_n(v) = \mathring{D}_n^{\alpha}(y,z)$$
$$(\text{when } n \text{ is odd}) = -P_n(v) - y\,Q_n(v) = -\mathring{D}_n^{\alpha}(y,z).$$

Thus we obtain

$$\mathring{D}_n^{-\alpha}(-y,z) = (-1)^n \mathring{D}_n^{\alpha}(y,z).$$

Similar arguments can be used to show the other equations in (5.10).

(iii) We have shown that $\{Q_n(v)\}$ and $\{P_n(v)\}$ are orthogonal polynomials by Favard's Theorem in Proposition 5. Following from the separation theorem for the zeros [5, Chapter I, Theorem 5.3], we know that the roots of $P_n(v)$ and $P_{n+1}(v)$ interlace, and the roots of $Q_n(v)$ and $Q_{n+1}(v)$ interlace.

In Proposition 5, we also showed that $Q_n(v)$ and $P_n(v)$ are related by the equation $-bP_{n-1}(v) = Q_n(v)$. Thus the roots of $Q_n(v)$ are the same as the roots of $P_{n-1}(v)$. The roots of $P_{n-1}(v)$ and the ones of $P_n(v)$ interlace by the separation theorem for the zeros. Thus it follows that the roots of $Q_n(v)$ and of $P_n(v)$ interlace, *i.e.*

$$v_{nk} < w_{nk} < v_{n,k+1}, \quad k = 1, 2, \ldots, n-1. \tag{5.11}$$

(iv) That the roots v of P_n and Q_n satisfy $|v| < b+1$ is proved by induction.

First, we prove monotonicity of the P_n at $b+1$, that is,

$$P_n(b+1) > P_{n-1}(b+1), \quad \text{for } n \geq 1.$$

This holds for $n = 1$, because $P_1(b+1) = b+1$, and $P_0(b+1) = 1$. Since $b > 0$, we have $P_1(b+1) > P_0(b+1)$. This is the base case for induction.

Now as the induction hypothesis, assume the inequality for a given value of $n \geq 1$. This means

$$b(P_n(b+1) - P_{n-1}(b+1)) > 0,$$

which implies

$$(b+1)P_n(b+1) - bP_{n-1}(b+1) > P_n(b+1).$$

Since the left-hand side of this latter inequality is equal to $P_{n+1}(b+1)$ by the recurrence relation, thus

$$P_{n+1}(b+1) > P_n(b+1).$$

Therefore,

$$P_n(b+1) > P_{n-1}(b+1), \text{ for } n \geq 1$$

is established by induction.

Next, we again use induction to prove that the roots v of P_n and Q_n satisfy $|v| < b+1$. Observe that the only root of P_1 is zero, we use this as our base case for induction. Then as the induction hypothesis, we assume at the largest root v_{nn} of P_n is less than $b+1$. Then since by Proposition 6(i), P_n is monic, we have $P_n(b+1) > 0$. From the recurrence relation and monotonicity of $\{P_n\}$ at $v = b+1$, we obtain

$$\begin{aligned} P_{n+1}(b+1) &= (b+1)P_n(b+1) - bP_{n-1}(b+1) \\ &> b\left(P_n(b+1) - P_{n-1}(b+1)\right) \\ &> 0. \end{aligned}$$

At $v = v_{nn}$, one obtains

$$\begin{aligned} P_{n+1}(v_{nn}) &= v_{nn}P_n(v_{nn}) - bP_{n-1}(v_{nn}) \\ &= -bP_{n-1}(v_{nn}) \\ &< 0. \end{aligned}$$

The last inequality above comes from the interlacing property that $v_{n-1,n-1} < v_{nn}$. Since the largest root of P_{n-1} is less than v_{nn} and P_{n-1} is monic, one has $P_{n-1}(v_{nn}) > 0$. The inequalities $P_{n+1}(v_{nn}) < 0$ and $P_{n+1}(b+1) > 0$ imply that P_{n+1} has a root v_* strictly between v_{nn} and $b+1$. Since the interlacing property implies that $v_{n+1,n} < v_{nn}$, the root v_* must be the largest root of P_{n+1}, that is $v_* = v_{n+1,n+1}$. This proves that the roots of P_{n+1} are less than $b+1$. The symmetry of the roots then implies that all of the roots are between $-(b+1)$ and $(b+1)$.

The interlacing property of the n–1 roots of Q_n with the n roots of P_n implies the analogous result for Q_n.

$\square$

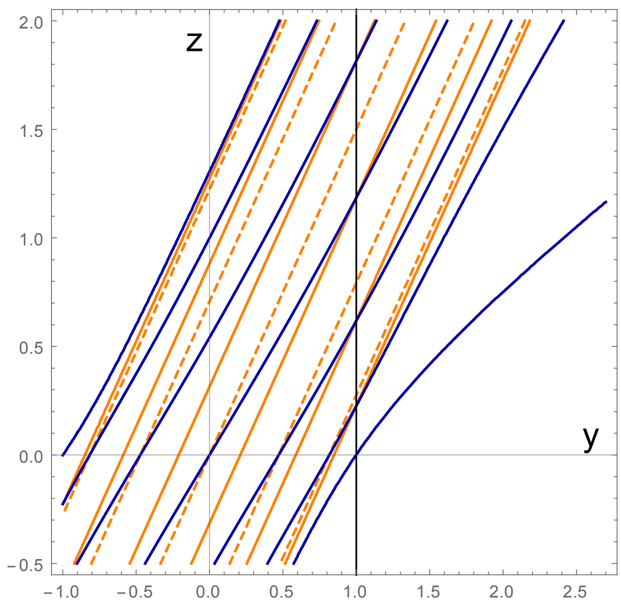

Figure 5.2. Solid straight lines: level sets of P_n. Dashed straight lines: level sets of Q_n. Solid curves: level sets of D_n.

Figure 5.2 illustrates how the straight-line zero sets of $P_n((b+1)y+\alpha z)$ and $Q_n((b+1)y+\alpha z)$ constrain the component curves of the zero set of $D_n(y,z)$ to lie in certain slanted strips. Two of these curves are unconstrained for $y>1$, and in fact, on these curves, the value of v becomes unbounded. They are responsible for the two rogue negative eigenvalues of the operator B_n that occur for large $\alpha<0$. Theorem 7 makes this observation precise and gives the asymptotic behavior of the two unconstrained component curves of $D_n(y,z)=0$.

Theorem 7. *(i) The zero set Z_n of D_n defined by $Z_n := \{(y,z)\in\mathbb{R}^2 : D_n(y,z)=0\}$, is invariant under the transformation $(y,z)\mapsto(-y,-z)$.*

(ii) The intersection of Z_n with the y-axis is

$$\{y\in\mathbb{R} : (y,0)\in Z_n\} = \{w_{nj}/(b+1) : 1\le j<n\}\cup\{-1,1\}\,. \tag{5.12}$$

For $\alpha \neq 0$, the intersection of Z_n with the line $y = 1$ is

$$\{z \in \mathbb{R} : (1, z) \in Z_n\} = \{(v_{nj} - (b+1))/\alpha : 1 \leq j \leq n\} \cup \{0\}\,. \tag{5.13}$$

(iii) The zero set Z_n of D_n consists of $n+1$ disjoint curves $\mathcal{C}_{nk}$ for $0 \leq k \leq n$. That is,

$$Z_n := \big\{(y, z) \in \mathbb{R}^2 : D_n(y, z) = 0\big\} = \bigcup_{k=0}^{n} \mathcal{C}_{nk}\,. \tag{5.14}$$

And each curve $\mathcal{C}_{nk}$ is the graph of an monotonic increasing function $y = g_{nk}(z)$.

(iv) For $\alpha < 0$ and $z \geq 0$, points $(y = g_{nk}(z), z) \in \mathcal{C}_{nk}$ are constrained to lie in the following slanted strips:

$$\begin{aligned}
k = 0 : &\quad \begin{cases} -(b+1) \leq \ (b+1)y + \alpha z \ \leq v_{n1} & \text{for } -1 \leq y \leq 1 \\[1em] v_{n1} \leq \ (b+1)y + \alpha z \ \leq w_{n1} & \text{for } 1 \leq y \end{cases} \\[2em]
k = 1, \ldots, n-2 : &\quad \begin{cases} w_{nk} \leq \ (b+1)y + \alpha z \ \leq v_{n,k+1} & \text{for } -1 \leq y \leq 1 \\[1em] v_{n,k+1} \leq \ (b+1)y + \alpha z \ \leq w_{n,k+1} & \text{for } 1 \leq y \end{cases} \\[2em]
k = n-1 : &\quad \begin{cases} w_{n,n-1} \leq \ (b+1)y + \alpha z \ \leq v_{nn} & \text{for } -1 \leq y \leq 1 \\[1em] v_{nn} \leq \ (b+1)y + \alpha z & \text{for } 1 \leq y \end{cases} \\[2em]
k = n : &\quad b+1 \leq \ (b+1)y + \alpha z \qquad\qquad \text{for } 1 \leq y\,.
\end{aligned} \tag{5.15}$$

Proof. (i) From Proposition 6 part (ii), we know that

$$D_n(-y, -z) = (-1)^{n+1} D_n(y, z).$$

Therefore, if $(y,z) \in Z_n := \{(y,z) \in \mathbb{R}^2 : D_n(y,z) = 0\}$, then $(-y,-z) \in Z_n$. As a result, in the following analysis, we may mainly consider the half y-z plane where $z \geq 0$.

(ii) From equation (5.8), we have

$$D_n(y,z) = \alpha z\, P_n(v) + (1-y^2)\, Q_n(v).$$

We continue to use $\{v_{nj}\}_{j=1}^{n}$ to denote the roots for $P_n(v)$, and $\{w_{nj}\}_{j=1}^{n-1}$ for the roots of $Q_n(v)$. When $z = 0$, we have $D_n(y,z) = (1-y^2)\, Q_n(v)$ with $v = \alpha z + (b+1)y$. Therefore, in the y-z plane, on the y-axis, the zero level sets of $D_n(y,z)$ coincide with the zero level sets of $Q_n(v)$, plus the points $y = 1$ and $y = -1$. Thus, the points on the intersection of Z_n with y-axis satisfies $\alpha z + (b+1)y = w_{nj}$, where $z = 0$. So on these intersection points, we have $y = w_{nj}/(b+1)$. Thus we can write the intersection of Z_n with y-axis as

$$\{y \in \mathbb{R} : (y,0) \in Z_n\} = \{w_{nj}/(b+1) : 1 \leq j < n\} \cup \{-1, 1\}. \qquad (5.16)$$

When $y = 1$, we have $D_n(y,z) = \alpha z\, P_n(v)$ with $v = \alpha z + (b+1)y$. That is, the zero level sets of $D_n(y,z)$ coincide with the zero level sets of $P_n(v)$, plus the point where $z = 0$. Thus, the points on the intersection of Z_n with the line $y = 1$ satisfies $\alpha z + (b+1)y = v_{nj}$, where $y = 1$. We obtain $z = (v_{nj} - (b+1))/\alpha$. Hence, for $\alpha \neq 0$, the intersection of Z_n with the line $y = 1$ is

$$\{z \in \mathbb{R} : (1,z) \in Z_n\} = \{(v_{nj} - (b+1))/\alpha : 1 \leq j \leq n\} \cup \{0\}. \qquad (5.17)$$

(iii) Because of the recursion relation for the sequence $\{D_n(y,z)\}_{n=-1}^{\infty}$ and Favard's Theorem, for fixed y this is a sequence of orthogonal polynomials in z (provided $\alpha \neq 0$), and for fixed z, this is a sequence of orthogonal polynomials in y. Since the roots of orthogonal polynomials are simple, it follows that for all (y, z) such that $D_n(y, z)$ is zero, both $\partial D_n/\partial z(y, z)$ and $\partial D_n/\partial y(y, z)$ must be nonzero. By the implicit function theorem, each component of the zero set of D_n in the yz-plane is a strictly monotonic function $y = g(z)$.

Also from part (ii) of this proof, we see that there are $n + 1$ intersection points of the zero set of D_n with the y-axis and the line $y = 1$. Hence we know that there are $n+1$ disjoint components in the zero set of D_n, and each of them is an increasing function. Thus we can call those disjoint curves C_{nk} for $0 \le k \le n$, and each C_{nk} is a monotonic increasing function $y = g_{nk}(z)$. We thus have

$$Z_n := \left\{(y, z) \in \mathbb{R}^2 : D_n(y, z) = D_n(g_{nk}(z), z) = 0\right\} = \bigcup_{k=0}^{n} \mathcal{C}_{nk} \, . \qquad (5.18)$$

(iv) We proved in Proposition 6 part (iii) that the roots of $\{P_n\}$ interlace with the roots of Q_n, which can be expressed as in equation (5.11):

$$v_{nk} < w_{nk} < v_{n,k+1}, \qquad k = 1, 2, \ldots, n-1.$$

We also have that

$$D_n(y, z) = \alpha z \, P_n(v) + (1 - y^2) \, Q_n(v).$$

For $\alpha < 0$, and $z \ge 0$, we analyze the points (y, z) on the zero level set Z_n of D_n with the cases when $-1 \le y \le 1$ and when $y \ge 1$.

When $\alpha < 0$, $z \ge 0$, and $-1 \le y \le 1$, we know that $\alpha z < 0$ and $1 - y^2 \ge 0$. Since $D_n(y, z) = \alpha z \, P_n(v) + (1 - y^2) \, Q_n(v)$, we see that $D_n(y, z) = 0$ when $P_n(v)$ and $Q_n(v)$ have the same sign, *i.e.*, when they are either both positive, or both negative. When $z = 0$ and $y = -1$, we have $(b+1)y + \alpha z = -(b+1)$, and we know that $y = g_{nk}(z)$ is monotonic increasing. Hence, for $k = 0$, the points (y, z) on the curve $\mathcal{C}_{n0}$ satisfy the inequality $-(b+1) \leq (b+1)y + \alpha z \leq v_{n1}$. For $k = 1, \ldots, n-1$, we have

$$w_{nk} \leq (b+1)y + \alpha z \leq v_{n,k+1} \quad \text{for} \quad -1 \leq y \leq 1.$$

When $\alpha < 0$, $z \geq 0$, and $y \geq 1$, we know $1 - y^2 \leq 0$. Thus $D_n(y, z) = 0$ when $P_n(v)$ and $Q_n(v)$ have opposite signs. Hence, for $k = n-1$, we have $\alpha z + (b+1)y \geq v_{nn}$; for $k = n$, we know that $(b+1)y + \alpha z = b+1$ when $z = 0$ and $y = 1$. Since $y = g_{nk}(z)$ is monotonic increasing, the points (y, z) on the curve $\mathcal{C}_{nn}$ satisfy that $(b+1)y + \alpha z \geq b+1$; and for $k = 0, \ldots, n-2$, we have

$$v_{n,k+1} \leq (b+1)y + \alpha z \leq w_{n,k+1} \quad \text{for} \;\; 1 \leq y.$$

We have shown in part (iv) Proposition (6) that the roots of P_n and the roots of Q_n lie between $-(b+1)$ and $(b+1)$. Thus the results of part (iv) follow.

$\square$

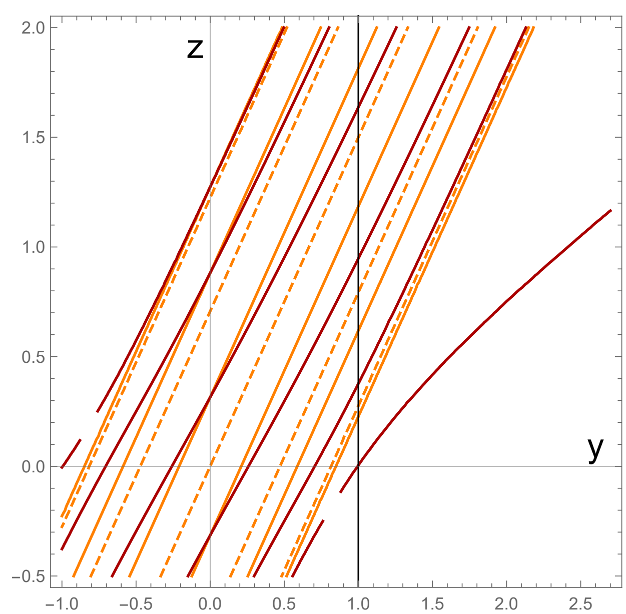

Figure 5.3. Solid straight lines: level sets of P_n. Dashed straight lines: level sets of Q_n. Solid curves: level sets of $\mathring{D}_n$.

Similarly, Figure 5.3 illustrates how the straight-line zero sets of $P_n((b+1)y+\alpha z)$ and $Q_n((b+1)y+\alpha z)$ constrain the component curves of the zero set of $\mathring{D}_n(y,z)$ to lie in certain slanted strips. One of these curves is unconstrained for $y>1$, and in fact, on this curve, the value of v becomes unbounded. The unconstrained curve is responsible for the one rogue negative eigenvalue of the operator $\mathring{B}_n$ that occur for large $\alpha<0$. Theorem 8 makes this observation precise and gives the asymptotic behavior of the one unconstrained component curve of $\mathring{D}_n(y,z)=0$.

Theorem 8. *(i) For $\alpha \neq 0$, the intersection of the zero set $\mathring{Z}_n$ with the line z-axis is*

$$\left\{z \in \mathbb{R} : (0,z) \in \mathring{Z}_n\right\} = \{v_{nj}/\alpha : 1 \le j \le n\}\,. \tag{5.19}$$

(ii) The zero set $\mathring{Z}_n$ of $\mathring{D}_n$ consists of n disjoint curves $\mathring{\mathcal{C}}_{nk}$ for $1 \le k \le n$,

$$\mathring{Z}_n := \left\{(y,z) \in \mathbb{R}^2 : \mathring{D}_n(y,z) = 0\right\} = \bigcup_{k=1}^{n} \mathring{\mathcal{C}}_{nk}\,, \tag{5.20}$$

and each curve $\mathring{\mathcal{C}}_{nk}$ is the graph of a monotonic function $y=\mathring{g}_{nk}(z)$.

(iii) These curves $\mathring{\mathcal{C}}_{nk}$ of $\mathring{Z}_n$ contain the following points on the z-axis:

$$\mathring{\mathcal{C}}_{nk} \;\supset\; \big(0, \frac{v_{nk}}{\alpha}\big) \qquad (1 \le k \le n).$$

(iv) If $(y,z) \in \mathring{\mathcal{C}}_{nk}$, then $(-y,-z) \in \mathring{\mathcal{C}}_{nk}$, that is, the functions g_{nk} are odd.

(v) For $\alpha \neq 0$ and $z \geq 0$, points $(y = g_{nk}(z), z) \in \mathring{\mathcal{C}}_{nk}$ are constrained to lie in the following slanted strips:

$$k = 1: \begin{cases} -(b+1) \leq & (b+1)y + \alpha z & \leq v_{n1} & \textit{for } y \leq 0 \\ v_{n1} \leq & (b+1)y + \alpha z & \leq w_{n1} & \textit{for } 0 \leq y \end{cases}$$

$$k = 2, \ldots, n-1: \begin{cases} w_{nk} \leq & (b+1)y + \alpha z & \leq v_{n,k+1} & \textit{for } y \leq 0 \\ v_{n,k+1} \leq & (b+1)y + \alpha z & \leq w_{n,k+1} & \textit{for } 0 \leq y \end{cases}$$

$$k = n: \begin{cases} w_{n,n-1} \leq & (b+1)y + \alpha z & \leq v_{nn} & \textit{for } y \leq 0 \\ b+1 \leq & (b+1)y + \alpha z & & \textit{for } 0 \leq y \end{cases} \tag{5.21}$$

Proof. (i) From Equation (5.8), we know that

$$\mathring{D}_n(y, z) = P_n(v) + y\, Q_n(v).$$

Thus, when $y = 0$, $\mathring{D}_n(y, z) = P_n(v)$ with $v = \alpha z + (b+1)y$. Therefore, in the yz plane, on the z-axis, the zero level sets of $\mathring{D}_n(y, z)$ concide with the zero level sets of $P_n(v)$. Thus, the points on the intersection of $\mathring{Z}_n$ with z-axis satisfies $\alpha z + (b+1)y = v_{nj}$, where $y = 0$. So on these intersection points, we have $z = \dfrac{v_{nj}}{\alpha}$, provided $\alpha \neq 0$. Thus we can write the intersection of $\mathring{Z}_n$ with z-axis as

$$\left\{ z \in \mathbb{R} : (0, z) \in \mathring{Z}_n \right\} = \left\{ v_{nj}/\alpha : 1 \leq j \leq n \right\}. \tag{5.22}$$

(ii) The argument to prove this part resembles the one for the previous theorem. Because of the recursion relation for the sequence $\{\mathring{D}_n(y, z)\}_{n=-1}^{\infty}$ and Favard's Theorem, for fixed y this is a sequence of orthogonal polynomials in z, and for fixed z, this is a sequence of orthogonal polynomials in y. Since the roots of orthogonal polynomials are simple, it follows that for all (y, z) such that $\mathring{D}_n(y, z)$ is zero, both $\partial\mathring{D}_n/\partial z(y, z)$ and $\partial\mathring{D}_n/\partial y(y, z)$ must be nonzero. By the implicit function theorem, each component of the zero set of $\mathring{D}_n$ in the yz-plane is a strictly monotonic function $y = g(z)$.

Also from part (i) of this proof, we see that there are n intersection points of the zero set of $\mathring{D}_n$ with the z-axis. Hence we know that there are n disjoint components in the zero set of $\mathring{D}_n$. We call those disjoint curves $\mathring{\mathcal{C}}_{nk}$ for $0 \leq k \leq n$, and each $\mathring{\mathcal{C}}_{nk}$ is a monotonic function $y = \mathring{g}_{nk}(z)$. We thus have

$$\mathring{Z}_n := \Big\{(y, z) \in \mathbb{R}^2 : \mathring{D}_n(y, z) = 0\Big\} = \bigcup_{k=1}^{n} \mathring{\mathcal{C}}_{nk}\,. \tag{5.23}$$

(iii) Combing the results from (i) and (ii), we obtain that These curves $\mathring{\mathcal{C}}_{nk}$ of $\mathring{Z}_n$ contain the following points on the z-axis:

$$\mathring{\mathcal{C}}_{nk} \quad \supset \quad \big(0, \frac{v_{nk}}{\alpha}\big) \qquad (1 \leq k \leq n).$$

(iv) From Proposition 6 part (ii), we know that

$$\mathring{D}_n(-y, -z) = (-1)^n \mathring{D}_n(y, z).$$

Therefore, if $(y, z) \in \mathcal{C}_{nk}$, then $(-y, -z) \in \mathring{\mathcal{C}}_{nk}$. That is, the functions $y = \mathring{g}_{nk}(z)$ is odd. As a result, in the following analysis, we may mainly consider the half y-z plane where $z \geq 0$.

(v) We proved in Proposition 6 part (iii) that the roots of $\{P_n\}$ interlace with the roots of Q_n, which can be expressed as in equation (5.11):

$$v_{nk} < w_{nk} < v_{n,k+1}, \qquad k = 1, 2, \ldots, n-1.$$

We also have that

$$\mathring{D}_n(y,z) = P_n(v) + y\,Q_n(v).$$

For $\alpha < 0$, and $z \geq 0$, we analyze the points (y,z) on the zero level set $\mathring{Z}_n$ of $\mathring{D}_n$ with the cases when $y \leq 0$ and when $y \geq 0$.

When $\alpha < 0$, $z \geq 0$, and $y \leq 0$, we see that $\mathring{D}_n(y,z) = 0$ when when $P_n(v)$ and $Q_n(v)$ have the same sign, *i.e.*, when they are either both positive, or both negative. Hence, when $k = 1$, points points (y,z) on the curves $\mathring{\mathcal{C}}_{n0}$ satisfy

$$(b+1)y + \alpha z \leq v_{n1} \quad \text{for } \; y \leq 0,$$

for $k = 2, \ldots, n$, the points (y,z) on the curves $\mathring{\mathcal{C}}_{nk}$ satisfy

$$w_{n,k-1} \leq (b+1)y + \alpha z \leq v_{n,k} \quad \text{for } \; y \leq 0.$$

When $\alpha < 0$, $z \geq 0$, and $y \geq 0$, . Thus $D_n(y,z) = 0$ when $P_n(v)$ and $Q_n(v)$ have opposite signs. Hence, for $k = 1, \ldots, n-1$, the points (y,z) on the curves $\mathring{\mathcal{C}}_{nk}$ satisfy

$$v_{n,k} \leq (b+1)y + \alpha z \leq w_{n,k} \quad \text{for } \; y \geq 0,$$

and for $k = n$, the points (y,z) on the curves $\mathring{\mathcal{C}}_{nn}$ satisfy

$$(b+1)y + \alpha z \geq v_{nn} \quad \text{for } \; y \geq 0.$$

We have shown in part (iv) Proposition (6) that the roots of P_n and the roots of Q_n lie between $-(b+1)$ and $(b+1)$. Thus the results of part (v) follow.

$\square$

Theorem 7 confirms Fig. 5.2, which illustrates that, for $z > 0$ and $\alpha \neq 0$, all but the right-most two component curves $\mathcal{C}_{nk}$ of $D_n(y,z) = 0$ are constrained to lie in slanted strips bounded by fixed values of $v = \alpha z + (b+1)y$ equal to roots of P_n and Q_n. The two unconstrained curves are asymptotically close to straight lines, as stated in Corollary 12.

Meanwhile, Theorem 8 confirms Fig. 5.3, which illustrates that, for $z > 0$ and $\alpha \neq 0$, all of the component curves of $\mathring{D}_n(y,z) = 0$, except for the right-most one, are constrained within slanted strips. Corollary 13 says that the one unconstrained curve $\mathring{\mathcal{C}}_{nn}$ is asymptotically close to the curve $\mathcal{C}_{nn}$.

Proposition 9. *The ratio of $P_{n+1}(v)$ and $Q_{n+1}(v)$ satisfies the equation*

$$\frac{-bP_{n+1}(v)}{vQ_{n+1}(v)} = 1 - v^{-2}\sum_{j=0}^{\infty} v^{-j}\int t^j d\psi_n(t) = 1 - v^{-2}\sum_{j=0}^{\infty} v^{-j}\mu_j^{(n)}, \tag{5.24}$$

where the integrals $\mu_j^{(n)} = \int t^j d\psi_n(t)$ are the moments of the approximating measures, and for $j \leqslant 2n-1$, we have

$$\mu_j^{(n)} = \int t^j d\psi_n(t) = \int t^j d\psi(t) = \mu_j \qquad (j \leqslant 2n-1).$$

Proof. We showed in Proposition 5 that $P_n(v)$ and $Q_n(v)$ are related by the equation $-bP_nv = Q_{n+1}(v)$, and the sequence $\{P_n(v)\}$ has a three-term recurrence relation $P_n(v) = vP_{n-1}(v) - bP_{n-1}(v)$. Thus we have

$$\begin{aligned}
\frac{-bP_{n+1}(v)}{vQ_{n+1}(v)} &= \frac{P_{n+1}(v)}{vP_n(v)} \\
&= \frac{vP_n(v) - bP_{n-1}(v)}{vP_n(v)} \\
&= 1 - \frac{bP_{n-1}(v)}{vP_n(v)} \\
&= 1 - \frac{1}{v}\sum_{k=1}^{n}\frac{A_{nk}}{v - v_{nk}} \quad \text{[5, Chapter III, Theorem 4.3]}
\end{aligned}$$

$$
\begin{aligned}
&= 1 - \frac{1}{v}\int_{-(b+1)}^{b+1} \frac{d\psi_n(t)}{v-t} \quad \text{(reference same as above)} \\
&= 1 - \frac{1}{v^2}\int_{-(b+1)}^{b+1} \frac{d\psi_n(t)}{1-tv^{-1}} \\
&= 1 - \frac{1}{v^2}\int_{-(b+1)}^{b+1} \sum_{j=0}^{\infty}(tv^{-1})^j d\psi_n(t) \\
&= 1 - v^{-2}\sum_{j=0}^{\infty} v^{-j}\int t^j d\psi_n(t) \\
&= 1 - v^{-2}\sum_{j=0}^{\infty} v^{-j}\mu_j^{(n)}.
\end{aligned}
$$

According to the Gauss quadrature formula [5, Chapter I, Theorem 6.1], for $j \leqslant 2n-1$, we have $\int t^j d\psi_n(t) = \int t^j d\psi(t) = \mu_j$. $\square$

Theorem 10. *If $b \geq 2$ and $\alpha \neq 0$, the two unconstrained components of the zero set of $D_n(y,z)$ and the one unconstrained component of $\mathring{D}_n(y,z)$ have the following asymptotic behavior as $y \to \infty$ in the yz-plane.*

$$
\alpha z = c_1^{(n)}y + c_0^{(n)} + c_{-1}^{(n)}y^{-1} + c_{-2}^{(n)}y^{-2} + c_{-3}^{(n)}y^{-3} + c_{-4}^{(n)}y^{-4} + \cdots + c_{-k}^{(n)}y^{-k} + \ldots,
$$

where, when k is odd, the coefficients c_{-k} depend on $\mu_0^{(n-1)}, \mu_2^{(n-1)}, \ldots, \mu_{k-1}^{(n-1)}$ and not on $\mu_j^{(n-1)}$ for $j \geq k$; when k is even, the coefficients c_{-k} depend on $\mu_0^{(n-1)}$, $\mu_2^{(n-1)}$, $\ldots$, $\mu_{k-2}^{(n-1)}$ and not on $\mu_j^{(n-1)}$ for $j \geq k-1$.

Proof. From equation (5.8), we see that $D_n(y,z)$ is related to $P_n(v)$ and $Q_n(v)$ through the equation

$$
D_n(y,z) = \alpha z P_n(v) + (1-y^2)Q_n(v).
$$

Thus $D_n(y,z) = 0$ is equivalent to

$$\frac{-bv\alpha z P_n(v)}{vQ_n(v)} - \frac{bv(1-y^2)Q_n(v)}{vQ_n(v)} = 0$$

$$v\alpha z\big(1 - v^{-2}\sum_{j=0}^{\infty} v^{-j}\int t^j d\psi_{n-1}(t)\big) - b(1-y^2) = 0$$

$$\alpha z v - \alpha z v^{-1}(\mu_0^{(n-1)} + v^{-1}\mu_1^{(n-1)} + v^{-2}\mu_2^{(n-1)} + v^{-3}\mu_3^{(n-1)} + \dots) - b + by^2 = 0. \tag{5.25}$$

Here $\mu_j^{(n-1)} = \int t^j d\psi_{n-1}(t)$. For $j \leq 2(n-1)-1$, that is for $j \leq 2n-3$, we have $\int t^j d\psi_{n-1}(t) = \int t^j d\psi_(t) = \mu_j$. Since we have discussed earlier that the odd terms of $\mu_j^{(n-1)}$ vanish. so the last of the above equations is equivalent to

$$\alpha z v - \alpha z v^{-1}\,(\,\mu_0^{(n-1)} + v^{-2}\mu_2^{(n-1)} + v^{-4}\mu_4^{(n-1)} + v^{-6}\mu_6^{(n-1)} + \dots) - b + by^2 = 0. \tag{5.26}$$

Suppose

$$\alpha z = c_1^{(n)} y + c_0^{(n)} + c_{-1}^{(n)} y^{-1} + c_{-2}^{(n)} y^{-2} + c_{-3}^{(n)} y^{-3} + c_{-4}^{(n)} y^{-4} + \dots + c_{-k}^{(n)} y^{-k} + \dots.$$

Then

$$\begin{aligned} v &= \alpha z + (b+1)y = (c_1^{(n)} + b + 1)y + c_0^{(n)} + c_{-1}^{(n)} y^{-1} + \\ &\quad + c_{-2}^{(n)} y^{-2} + c_{-3}^{(n)} y^{-3} + c_{-4}^{(n)} y^{-4} + \dots + c_{-k}^{(n)} y^{-k} + \dots. \end{aligned}$$

Let $y^{-1} = \eta$, $\gamma_1 = c_1^{(n)} + b + 1$, and $\gamma_l = c_{-l}^{(n)}$ for $l \geq 0$. Then we can write $v = \sum_{l=-1}^{\infty} \gamma_l \eta^l$. We suppose $v^{-1} = \sum_{k=1}^{\infty} \delta_k \eta^k$. Since $vv^{-1} = 1$, we have

$$vv^{-1} = \sum_{n=0} \eta^n \sum_{l+k=n} \gamma_l \delta_k = \sum_{n=0} \eta^n \sum_{l=-1}^{n-1} \gamma_l \delta_{n-l} = 1.$$

So to find the coefficients δ_k for v^{-1}, we have

$$\begin{aligned}
\text{When } n=0 &\;:\; \gamma_{-1}\delta_1 = 1 \\
\text{When } n=1 &\;:\; \gamma_{-1}\delta_2 + \gamma_0\delta_1 = 0 \\
\text{When } n=2 &\;:\; \gamma_{-1}\delta_3 + \gamma_0\delta_2 + \gamma_1\delta_1 = 0 \\
&\;\vdots \\
\text{Arbitrary } n &\;:\; \gamma_{-1}\delta_{n+1} + \sum_{l=0}^{n-1}\gamma_l\delta_{n-l} = 0\,.
\end{aligned}$$

So we have $\delta_{n+1} = -\frac{1}{\gamma_{-1}}\sum_{k=1}^{n}\gamma_{n-k}\delta_k$. Therefore, δ_{n+1} depends on γ_{-1}, γ_0, γ_1, $\ldots$, up to γ_{n-1}. Now we put everything into equation (5.26). Since the right hand side of the equation is equal to 0, the vanishing of the coefficients of y^{-k} $(k \geq -2)$ allows us to find $c_{-k}^{(n)}$ for $k \geq -1$. From the y^2 term, we find that

$$c_1^{(n)} = -b \quad \text{or} \quad c_1^{(n)} = -1\,. \tag{5.27}$$

In either case, the vanishing of the y term implies

$$c_0^{(n)} = 0 \quad \text{since} \quad b \neq 1\,. \tag{5.28}$$

The vanishing of the constant term allows us to find $c_{-1}^{(n)}$, but we also see that it involves $\mu_0^{(n-1)}$ because of the constant term in $\mu_0^{(n-1)}\alpha z v^{-1}$.

The vanishing of the coefficient of y^{-1} allows us to find $c_{-2}^{(n)}$, we see that it also involves $\mu_0^{(n-1)}$ because of the y^{-1} term in $\mu_0^{(n-1)}\alpha z v^{-1}$.

The vanishing of the coefficient of y^{-2} allows us to find $c_{-3}^{(n)}$, we see that it also involves $\mu_0^{(n-1)}$ and $\mu_2^{(n-1)}$ because of the y^{-2} term in $\mu_0^{(n-1)}\alpha z v^{-1}$ and $\mu_2^{(n-1)}\alpha z v^{-3}$.

If we continue our analysis like this, we find out, by induction, that $c_{-k}^{(n)}$ depends on $\mu_0^{(n-1)}, \mu_2^{(n-1)}, \ldots,$ up to $\mu_{k-1}^{(n-1)}$ when k is odd, and c_{-k} depends on $\mu_0^{(n-1)}, \mu_2^{(n-1)}, \ldots,$ up to $\mu_{k-2}^{(n-1)}$ when k is even.

Similarly, $\mathring{D}_n(y,z)$ is related to $P_n(v)$ and $Q_n(v)$ through the equation $\mathring{D}_n(y,z) = P_n(v) + yQ_n(v)$. Thus $\mathring{D}_n(y,z) = 0$ is equivalent to

$$\begin{aligned} \frac{-bvP_n(v)}{vQ_n(v)} - \frac{bvyQ_n(v)}{vQ_n(v)} &= 0 \\ v\big(1 - v^{-2}\sum_{j=0}^{\infty} v^{-j}\int t^j d\psi_{n-1}(t)\big) - by &= 0 \qquad (5.29) \\ v - v^{-1}(\mu_0^{(n-1)} + v^{-1}\mu_1^{(n-1)} + v^{-2}\mu_2^{(n-1)} + v^{-3}\mu_3^{(n-1)} + \dots) - by &= 0. \end{aligned}$$

The last equation above again simplifies to

$$v - v^{-1}\,(\,\mu_0^{(n-1)} + v^{-2}\mu_2^{(n-1)} + v^{-4}\mu_4^{(n-1)} + v^{-6}\mu_6^{(n-1)} + \dots) - by = 0, \qquad (5.30)$$

because of the vanishing of odd terms of $\mu_j^{(n-1)}$.

We again suppose

$$\alpha z = c_1^{(n)}y + c_0^{(n)} + c_{-1}^{(n)}y^{-1} + c_{-2}^{(n)}y^{-2} + c_{-3}^{(n)}y^{-3} + c_{-4}^{(n)}y^{-4} + \cdots + c_{-k}^{(n)}y^{-k} + \dots.$$

We put the above equation with $v = \alpha z + (b+1)y$ into equation (5.30). With similar analysis of comparing the coefficients of y^{-k}, we find that $c_1 = -1$, $c_0 = 0$, and the same results of the dependence of $c_{-k}^{(n)}$ on $\mu_j^{(n-1)}$. □

Corollary 11. *If $n_1 \neq n_2$, then the rogue zero sets $\mathcal{C}_{n_1n_1}$ of $D_{n_1}(y,z)$ and $\mathcal{C}_{n_2n_2}$ of $D_{n_2}(y,z)$ do not coincide. Similarly, $\mathcal{C}_{n_1,n_1-1}$ of $D_{n_1}(y,z)$ and $\mathcal{C}_{n_2,n_2-1}$ of $D_{n_2}(y,z)$ do not coincide. In addition, $\mathring{\mathcal{C}}_{n_1n_1}$ of $\mathring{D}_{n_1}(y,z)$ and $\mathring{\mathcal{C}}_{n_2n_2}$ of $\mathring{D}_{n_2}(y,z)$ do not coincide. Meanwhile, $\mathring{\mathcal{C}}_{n_1n_1}$ of $\mathring{D}_{n_1}(y,z)$ and $\mathcal{C}_{n_1n_1}$ of $D_{n_1}(y,z)$ do not coincide.*

Proof. From earlier discussion, we know that $\mu_j^{(n-1)} = \mu_j$ for $j \leq 2n-3$, *i.e.* for $n \geq \dfrac{j+3}{2}$. Suppose $n_1 = \dfrac{k+1}{2}$ for k is odd [or $\dfrac{k}{2}$ for k is even], and $n_2 \geq \dfrac{k+2}{2}$, then $\mu_l^{(n_2-1)} = \mu_l$ for $l \leq k-1$. but $\mu_{k-1}^{(n_1-1)} \neq \mu_{k-1}$ and $\mu_l^{(n_2-1)} = \mu_l$ for $l \leq k-2$. Therefore $c_{-k}^{(n_1)} \neq c_{-k}^{(n_2)}$. Similar arguments can show that the same is true for all the three cases in the statement of the corollary. □

Corollary 12. *If $b \geq 2$ and $\alpha \neq 0$, the two unconstrained components of the zero set of $D_n(y,z)$ have the following asymptotic behavior as $y \to \infty$ in the yz-plane.*

$$\begin{aligned} \mathcal{C}_{n,n-1} &: \quad \alpha z + b\,y - b\,y^{-1} + O(y^{-2}) = 0 \quad (y \to \infty) \\ \mathcal{C}_{nn} &: \quad \alpha z + y - y^{-1} + O(y^{-2}) = 0 \qquad (y \to \infty). \end{aligned} \tag{5.31}$$

Proof. From this and the relation $D_n(y,z) = \alpha z P_n(v) + (1-y^2)Q_n(v)$, the condition $D_n(y,z) = 0$ becomes

$$\begin{aligned} \alpha z P_n(v) + (1-y^2)Q_n(v) &= 0 \\ \frac{-bv\alpha z P_n(v)}{vQ_n(v)} - \frac{bv(1-y^2)Q_n(v)}{vQ_n(v)} &= 0. \end{aligned} \tag{5.32}$$

Here we use the result from Proposition (9) and Equation (5.5) and obtain

$$\begin{aligned} v\alpha z(1 - \mu_0 v^{-2} + O(v^{-4})) - b(1-y^2) &= 0 \\ v\alpha z(1 - bv^{-2} + O(v^{-4})) - b(1-y^2) &= 0 \\ \alpha z v - b\alpha\, z v^{-1} + z\,O(v^{-3}) + b\,y^2 - b &= 0\,. \end{aligned} \tag{5.33}$$

In the proof of Theorem 10, we were able to find c_{-1} and c_0. With a little more work in that proof, we were also able to obtain c_1. But we choose to present the calculation of c_{-1}, c_0, and c_1 in a self-contained way here.

Let us assume, for $v \to \infty$, solutions of the form

$$\alpha z = c_1 y + c_0 + c_{-1} y^{-1} + O(y^{-2}) \qquad (y \to \infty). \tag{5.34}$$

Recall that $v = \alpha z + (b+1)y$. The condition $c_1 > -(b+1)$ guarantees that $v \to \infty$ as $y \to \infty$. With the ansatz (5.34), one obtains

$$\alpha z v = c_1(c_1+b+1)y^2 + c_0(2c_1+b+1)y + 2c_1c_{-1} + c_0^2 + c_{-1}(b+1) + O(y^{-1})\,,$$

$$\alpha z v^{-1} = c_1(c_1+b+1)^{-1} + c_0(b+1)(c_1+b+1)^{-2}y^{-1} + O(y^{-2})\,.$$

Inserting these into the last equation of (5.33) yields

$$
\begin{aligned}
&[c_1(c_1+b+1)+b]\,y^2 + c_0\,(2c_1+b+1)\,y - bc_1(c_1+b+1)^{-1} - b + 2c_1c_{-1} + c_0^2 \\
&+ c_{-1}(b+1) - c_0 b(b+1)(c_1+b+1)^{-2}y^{-1} + O(y^{-2}) + zO(y^{-3}) \\
&= 0.
\end{aligned}
$$

Thus we can write

$$
\begin{gathered}
[c_1(c_1+b+1)+b]\,y^2 + c_0\,(2c_1+b+1)\,y + \\
-bc_1(c_1+b+1)^{-1} - b + 2c_1c_{-1} + c_0^2 + c_{-1}(b+1) = O(y^{-1})\,.
\end{gathered}
$$

The vanishing of the y^2 term implies

$$
c_1 = -b \quad \text{or} \quad c_1 = -1\,. \tag{5.35}
$$

In either case, the vanishing of the y term implies

$$
c_0 = 0 \quad \text{since} \quad b \neq 1\,. \tag{5.36}
$$

The vanishing of the constant term yields

$$
c_{-1} = \frac{b\,[1 + c_1(c_1+b+1)^{-1}]}{2c_1+b+1}\,, \tag{5.37}
$$

which equals b when $c_1 = -b$ and equals 1 when $c_1 = -1$. Since both possible values of c_1 satisfy $c_1 > -(b+1)$, one obtains asymptotic solutions of (5.33) of the form (5.34) as $v \to \infty$. These necessarily coincide with the curves $\mathcal{C}_{n,n-1}$ and $\mathcal{C}_{nn}$ because, according to Theorem 7, the value of v remains bounded on the curves $\mathcal{C}_{nk}$ for $k < n-1$.

When $c_1 = -b$, $c_0 = 0$, $c_{-1} = b$, and when $c_1 = -1$, $c_0 = 0$, $c_{-1} = 1$, we insert into the assumption equation 5.34 and obtain the asymptotic behavior of the two unconstrained components of the zero sets of $D_n(y,z)$ as $y \to \infty$ in the yz plane as

$$\begin{aligned}
\mathcal{C}_{n,n-1} \ &: \ \alpha z + b\,y - b\,y^{-1} + O(y^{-2}) = 0 \quad (y \to \infty), \\
\mathcal{C}_{nn} \ &: \ \alpha z + y - y^{-1} + O(y^{-2}) = 0 \qquad (y \to \infty).
\end{aligned}$$

$\square$

Corollary 13. *If $\alpha \neq 0$, the one unconstrained component of the zero set of $\mathring{D}_n(y,z)$ has the following asymptotic behavior as $y \to \infty$ in the yz-plane.*

$$\mathring{\mathcal{C}}_{nn} \ : \ \alpha z + y - y^{-1} + O(y^{-2}) = 0 \qquad (y \to \infty). \tag{5.38}$$

Proof. Again using the result from Proposition (9) and Equation (5.5), we have

$$\frac{-bP_n(v)}{vQ_n(v)} = 1 - \mu_0 v^{-2} + O(v^{-4}) = 1 - bv^{-2} + O(v^{-4}).$$

Since

$$\mathring{D}_n(y,z) = P_n(v) + yQ_n(v),$$

the condition $\mathring{D}_n(y,z) = 0$ becomes

$$v - bv^{-1} + O(v^{-3}) - by \ = \ 0 \qquad (v \to \infty)\,. \tag{5.39}$$

Again we assume, for $v \to \infty$, the solutions are of the form

$$\alpha z = c_1 y + c_0 + c_{-1} y^{-1} + O(y^{-2}) \qquad (y \to \infty). \tag{5.40}$$

Recall that $v = \alpha z + (b+1)y$. The condition $c_1 > -(b+1)$ guarantees that $v \to \infty$ as $y \to \infty$. Inserting $v = \alpha z + (b+1)y$ and equation (5.40) into equation (5.39), after simplification we obtain

$$(c_1+1)y + c_0 + \left(c_{-1} - b(c_1+b+1)^{-1}\right) y^{-1} + O(y^{-2}) \ = \ 0 \qquad (y \to \infty)\,. \tag{5.41}$$

This implies $c_1 = -1$, $c_0 = 0$, and $c_{-1} = 1$. Using ansatz (5.40), we obtain the desired equation

$$\alpha z + y - y^{-1} + O(y^{-2}) = 0 \qquad (y \to \infty).$$

This resulting curve must coincide with $\mathring{\mathcal{C}}_{nn}$ because, according to Theorem 8, the value of v remains bounded on the curves $\mathring{\mathcal{C}}_{nk}$ for $k < n$. $\square$

5.2 The curve $\mathcal{S}$

Analysis of the spiral curve $\mathcal{S}$, parameterized by $(c(\lambda), s(\lambda))$ relies on the asymptotics of the solutions of the Schrödinger equation on the interval $[0, 1]$. According to [7, Theorem 1.3.1], there is a continuous integral kernel K that realizes $c(x, \lambda)$ as a transformation of $\cos(\sqrt{\lambda}\, x)$:

$$c(x,\lambda) \;=\; \cos(\rho x) + \int_0^x K(x,y)\cos(\rho y)dy \qquad (\lambda = \rho^2). \tag{5.42}$$

The diagonal of K is

$$K(x,x) \;=\; \tfrac{1}{2}\int_0^x q(y)\,dy. \tag{5.43}$$

This implies an asymptotic correction [7, (1.1.9)] to $c(1, \lambda) = c(\lambda)$,

$$c(\lambda) \;=\; \cos\rho + O\big(\,|\rho|^{-1}\,e^{|\mathrm{Im}\rho|}\big) \qquad (|\lambda = \rho^2| \to \infty). \tag{5.44}$$

For $\lambda = -\nu^2$, or $\rho = i\nu$, the second term of (5.42) at $x = 1$ is

$$\begin{aligned}\int_0^1 K(1,y)\cosh(\nu y)dy \;&=\; \tfrac{1}{2}e^{\nu}\int_0^1 K(1,y)\big(e^{-\nu(1-y)} + e^{-\nu(1+y)}\big)dy \\ &= \tfrac{1}{2}e^{\nu}K(1,1)\nu^{-1} + e^{\nu}O(\nu^{-2}) \qquad (\lambda = -\nu^2,\ \nu^2 \to \infty).\end{aligned} \tag{5.45}$$

From this, one obtains the first two terms of an asymptotic expansion of $c(\lambda)$,

$$c(\lambda) \;=\; \tfrac{1}{2}e^{\nu}\big(1 + q_0\nu^{-1} + O(\nu^{-2})\big) \qquad (\lambda = -\nu^2,\ \nu^2 \to \infty), \tag{5.46}$$

in which

$$q_0 := K(1,1) = \tfrac{1}{2}\int_0^1 q(y)\,dy\,. \tag{5.47}$$

Similarly, [7, Theorem 1.3.2] writes $s(x, \lambda)$ as a transformation of $\sin(\rho x)/\rho$,

$$s(x,\lambda) \;=\; \frac{\sin(\rho x)}{\rho} + \int_0^x P(x,y)\frac{\sin(\rho y)}{\rho}dy, \tag{5.48}$$

with diagonal

$$P(x,x) \;=\; \tfrac{1}{2}\int_0^x q(y)\,dy. \tag{5.49}$$

This implies the asymptotic relation

$$s(\lambda) \;=\; \frac{\sin\rho}{\rho} + O\big(\,|\rho|^{-2}\,e^{|\mathrm{Im}\rho|}\big) \qquad (|\lambda=\rho^2|\to\infty). \tag{5.50}$$

For $\lambda=-\nu^2$, the second term (5.48) at $x=1$ produces

$$\begin{aligned}\nu^{-1}\int_0^1 P(1,y)\sinh(\nu y)dy \;&=\; \tfrac{1}{2}\nu^{-1}e^{\nu}\int_0^1 P(1,y)\big(e^{-\nu(1-y)}-e^{-\nu(1+y)}\big)dy\\ &= \tfrac{1}{2}\nu^{-2}e^{\nu}P(1,1)+e^{\nu}O(\nu^{-3}) \qquad (\lambda=-\nu^2,\,\nu^2\to\infty).\end{aligned} \tag{5.51}$$

The first two terms of an asymptotic expansion of $s(\lambda)$ are thus

$$s(\lambda) \;=\; \tfrac{1}{2}\nu^{-1}e^{\nu}\big(1+q_0\nu^{-1}+O(\nu^{-2})\big) \qquad (\lambda=-\nu^2,\,\nu^2\to\infty), \tag{5.52}$$

since again, $P(1,1)=q_0$.

5.3 Eigenvalues of the quantum-tree operator

We will see in this section that the eigenvalues of B_n and the eigenvalues of $\mathring{B}_n$ come in a countable number of groups, which we call bands (although they are not continuous). These bands will be denoted by Σ_k^n for B_n and by $\mathring{\Sigma}_k^n$ for $\mathring{B}_n$ for $k=0,1,2,\dots$. We enumerate in decreasing order the eigenvalues of the 0-th band Σ_0^n and $\mathring{\Sigma}_0^m$ as follows,

$$\lambda_{nn} \;<\; \lambda_{n,n-1} \;<\; \dots \;<\; \lambda_{n1} \;<\; \lambda_{n0}$$

$$\mathring{\lambda}_{mm} \;<\; \mathring{\lambda}_{m,m-1} \;<\; \dots \;<\; \mathring{\lambda}_{m2} \;<\; \mathring{\lambda}_{m1}\,.$$

In Theorem 7, we showed that the zero set Z_n of D_n consists of $n+1$ disjoint curves $\mathcal{C}_{nk}$ for $0\le k\le n$. We also showed in this theorem that for $z\ge 0$ and $\alpha<0$, points $(y=g_{nk}(z),z)$ of the "first" $n-1$ components are constrained to lie in the slanted strip

$$-(b+1)\le v_{n1}\le (b+1)y+\alpha z\le w_{n,n-1}\le b+1\,.$$

Thus the equations for the upper and lower constraining slanted lines are

$$\alpha z + (b+1)y + (b+1) = 0 \tag{5.53}$$

$$\alpha z + (b+1)y - (b+1) = 0. \tag{5.54}$$

On the parametric curve, the red part in the figure spirals at multiples of π for $q(x) = 0$ and asymptotically as $\lambda \to \infty$ at multiples of π in general, while the brown part is where $\lambda < 0$ are negative where it becomes a parametric curve of hyperbolic sine and hyperbolic cosine as $\lambda \to -\infty$. The intersections of the zero level sets and the parametric curve produce the spectrum of the quantum tree. In Figure 5.4 the spiral curve is the parametric curve of $(y, z) = (c(\lambda), s(\lambda)) = (\cos(\sqrt{\lambda}), \sin(\sqrt{\lambda})/\sqrt{\lambda})$ when $q(x) = 0$.

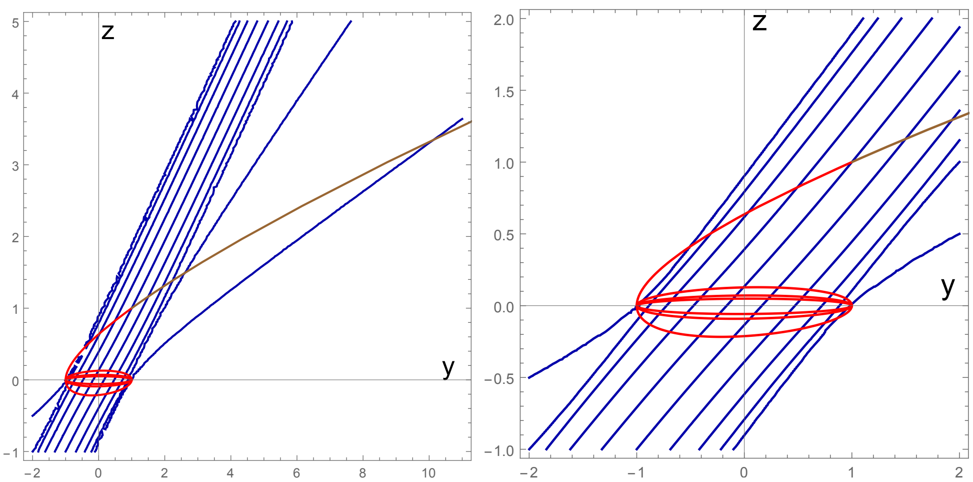

Figure 5.4. The blue curves are $\mathcal{C}_{nk}$, the zero level sets of $D_n(y, z)$. The spiral curves in red and brown are parametric curves of $y = c(\lambda)$, $z = s(\lambda)$ when the potential $q(x) = 0$.

The blue curves in Figure 5.4 are the zero level sets $\mathcal{C}_{nk}$ of $D_n(y, z)$. They seem almost to be straight lines, but actually they are not. Because the initial conditions for the three-term recurrence relation $D_n(v)$, where $v = (b+1)y + \alpha z$, depend on y and z instead of being constant. However, we have shown that each of the curves $\mathcal{C}_{nk}$ is monotonic increasing. Each intersection with the spiral curve $\mathcal{S}$ gives us an eigenvalue in the spectrum. The intersections of $\mathcal{S}$ with the $\mathcal{C}_{nk}$ give us the spectrum that are in spectral bands, where except the first band, each band is bounded below by $n^2\pi^2$ for the case when the potential $q(x) = 0$. For arbitrary potential $q(x)$, the spectral bands Σ_k^n $(k = 1, 2, \dots, n)$ for higher eigenvalues are displayed in Theorem 14. However, as we can tell from Figure 5.4, the 0-th band Σ_0^n includes negative or positive eigenvalues for $q(x) = 0$ depending on the slope of the zero curves $\mathcal{C}_{nk}$. When the slopes are small enough, which is equivalent to when α is negative large enough, the whole first band consists of negative eigenvalues. Actually from Equation (5.53), we can see that when $-\dfrac{b+1}{\alpha} < \dfrac{1}{2}$, *i.e.*, when $\alpha < -2(b+1)$, the first band is completely negative. This is included in Theorem 14.

More interestingly, we see there are two curves $\mathcal{C}_{n,n-1}$ and $\mathcal{C}_{nn}$ in the zero level sets of D_n straying away from the first band. We conclude that the negative eigenvalues λ for large negative α consist of one band of $n-1$ eigenvalues plus two rogue eigenvalues. Determining these eigenvalues as $\alpha \to -\infty$ requires finding the asymptotic relation between λ and α at the intersection points of the curve $(y, z) = (c(\lambda), s(\lambda))$ with asymptotically straight lines of the zero level sets in the yz-plane.

Theorem 14. *There exists a sequence $\lambda_1^*, \lambda_2^*, \dots, \lambda_k^*, \dots,$ tending to ∞, where $s(\lambda_k^*) = 0$ (depending on the potential q), such that, for each α and b, (Λ_n, B_n) has $n+1$ eigenvalues between λ_k^* and λ_{k+1}^*, and $(\Lambda_n, \mathring{B}_n)$ has n eigenvalues between λ_k^* and λ_{k+1}^*.*

Proof. From Equation (5.50), we see that for $\rho > 0$,

$$\rho s(\rho^2) = \sin\rho + O(\frac{1}{\rho}) \quad (\rho \to \infty).$$

Thus there exist constants C and ρ_0 such that when $\rho > \rho_0$, $|O(\dfrac{1}{\rho})| < C\dfrac{1}{\rho} < 1$. Since $\rho(\sin(\rho^2))$ is continuous, when $\rho > \rho_0$, for all integers $l > 0$,

$$\begin{cases} \quad \text{at } \rho = \dfrac{\pi}{2} + 2l\pi, \quad \sin\rho = 1, \qquad \text{so } \rho\, s(\rho^2) > 0 \\ \text{at } \rho = -\dfrac{\pi}{2} + 2l\pi, \quad \sin\rho = -1, \quad \text{so } \rho\ s(\rho^2) < 0. \end{cases} \tag{5.55}$$

Since $s(\rho^2)$ is analytic, so it has finitely many roots in the intervals $(-\frac{\pi}{2}+2l\pi, \frac{\pi}{2}+2l\pi))$. This establishes the sequences $\lambda_1^*, \lambda_2^*, \ldots, \lambda_k^*, \ldots$ of roots of s tending to ∞. These roots do not depend on α or b, since s depends only on q. For these roots $(\rho_k^*)^2$, from equation (5.44), we see that $c(\lambda_k^*)$ is approximately bounded between -1 and 1, with error $O(\frac{1}{\rho})$. In Theorem 7, we showed that the zero level set Z_n of $D_n(\lambda)$ has $n+1$ disjoint components $\mathcal{C}_{nk}$ for $0 \le k \le n$, where their intersections with the $y = c(\lambda)$-axis are

$$\{y \in \mathbb{R} : (y, 0) \in Z_n\} = \{w_{nj}/(b+1) : 1 \le j < n\} \cup \{-1, 1\}\,, \tag{5.56}$$

where w_{nj} are the roots of orthogonal polynomial $Q_n(v)$ for $v = (b+1)y + \alpha z$. We also showed in part (iv) of Proposition 6 that the roots of $Q_n(v)$ lie between $-(b+1)$ and $(b+1)$. Thus the intersections of Z_n with the y-axis lie in the interval $[-1, 1]$. Hence, for l large enough, Z_n intersects with the parametric curve $(c(\lambda), s(\lambda))$ $n+1$ times in each l-th interval $(-\frac{\pi}{2}+2l\pi, \frac{\pi}{2}+2l\pi))$, producing $n+1$ eigenvalues.

Similarly, in Theorem 8, we showed that the zero level set $\mathring{Z}_n$ of $\mathring{D}_n$ consists of n disjoint curves $\mathring{\mathcal{C}}_{nk}$ for $1 \le k \le n$. We know that their intersections with the y-axis are also in the interval $[-1, 1]$. Thus $(\Lambda_n, \mathring{B}_n)$ has n eigenvalues between λ_k^* and λ_{k+1}^*.

When $q = 0$, we know that $s(\rho^2) = \sin(\rho)/\rho$, and $c(\rho^2) = \cos(\rho)$. From Equation (5.53), we see that the slope of the upper constraining slanted line is $-\dfrac{b+1}{\alpha}$ on the yz-plane. Thus when $-\dfrac{b+1}{\alpha} < \dfrac{1}{2}$, which is equivalent to when $\alpha < -2(b+1)$, the first band Σ_0^n is completely negative. $\square$

Lemma 15. *For $c > 0$, $\lambda = -\nu^2$, there exists a relation*

$$\nu \;=\; -c^{-1}\alpha + O(\alpha^{-1}) \qquad (\alpha \to -\infty). \tag{5.57}$$

between α and ν, on which the curve

$$(y, z) = (c(\lambda), s(\lambda)) \tag{5.58}$$

satisfies

$$\alpha z + cy + v_0 + O(y^{-1}) \;=\; 0 \qquad (y \to \infty). \tag{5.59}$$

When $q(x) \equiv 0$, this value of ν can be refined to

$$\nu \;=\; -c^{-1}\alpha + c^{-2}v_0\,\alpha\, e^{c^{-1}\alpha} + O(\alpha\, e^{2c^{-1}\alpha}) \qquad (\alpha \to -\infty). \tag{5.60}$$

Proof. From the discussion of the previous section, one has

$$y \;=\; c(\lambda) \;=\; \tfrac{1}{2}\left(1 + q_0\,\nu^{-1} + O(\nu^{-2})\right) e^{\nu} \qquad (\nu \to \infty), \tag{5.61}$$

$$z \;=\; s(\lambda) \;=\; \tfrac{1}{2}\nu^{-1}\left(1 + q_0\,\nu^{-1} + O(\nu^{-2})\right) e^{\nu} \qquad (\nu \to \infty). \tag{5.62}$$

With the curve $(y, z) = (c(\lambda), s(\lambda))$ and the two equations above, the equation

$$\alpha z + cy + v_0 + O(y^{-1}) \;=\; 0 \qquad (y \to \infty) \tag{5.63}$$

becomes

$$\alpha\nu^{-1}\left(1 + q_0\,\nu^{-1} + O(\nu^{-2})\right) e^{\nu} + c\left(1 + q_0\,\nu^{-1} + O(\nu^{-2})\right) e^{\nu} + 2v_0 + O(y^{-1}) = 0$$

$$(\nu \to \infty,\ y \to \infty),$$

which implies that

$$(\alpha\nu^{-1} + c)\left(1 + q_0\,\nu^{-1} + O(\nu^{-2})\right) + O(e^{-\nu}) = 0 \qquad (\nu \to \infty).$$

Suppose $\alpha = c_1\nu + c_0 + c_{-1}\nu^{-1} + \ldots$; then we obtain

$$\left(c_1 + c_0\nu^{-1} + c_{-1}\nu^{-2} + c\right)\left(1 + q_0\,\nu^{-1} + O(\nu^{-2})\right) + O(e^{-\nu}) = 0 \qquad (\nu \to \infty),$$

which implies that

$$c + c_1 + ((c + c_1)q_0 + c_0\alpha)\,\nu^{-1} + O(\nu^{-2}) \;=\; 0 \qquad (\nu \to \infty),$$

whence $c_1 = -c$ and $c_0 = 0$ and hence $\alpha = -c\nu + O(\nu^{-1})$ as $\nu \to \infty$. This implies

$$\nu \;=\; -c^{-1}\alpha + O(\alpha^{-1}) \qquad (\alpha \to -\infty).$$

In the case that $q(x) \equiv 0$, one has

$$c(\lambda) \;=\; \tfrac{1}{2}\left(e^{\nu} + e^{-\nu}\right), \tag{5.64}$$

$$s(\lambda) \;=\; \tfrac{1}{2}\,\nu^{-1}\left(e^{\nu} - e^{-\nu}\right), \tag{5.65}$$

and thus obtains from equation (5.63) the α-ν relation

$$\alpha\nu^{-1} + c + v_0 e^{-\nu} + O(e^{-2\nu}) = 0 \qquad (\nu \to \infty),$$

which yields $\alpha = -c\nu - v_0\nu e^{-\nu} + O(\nu e^{-2\nu}) \qquad (\nu \to \infty)$ and hence (5.60)

$$\nu \;=\; -c^{-1}\alpha + c^{-2}v_0\,\alpha\, e^{c^{-1}\alpha} + O(\alpha\, e^{2c^{-1}\alpha}) \qquad (\alpha \to -\infty).$$

□

Theorem 16. *(Large negatives eigenvalues for $\alpha \to -\infty$) As $\alpha \to -\infty$, the two rogue eigenvalues for (Λ_n, B_n) satisfy*

$$\lambda_{nn} = -\nu^2 = -\alpha^2 + O(1) \qquad (\alpha \to -\infty)$$

$$\lambda_{n,n-1} = -\nu^2 = -b^{-2}\alpha^2 + O(1) \qquad (\alpha \to -\infty).$$

The other eigenvalues in the first band Σ_0^n satisfy

$$\lambda_{nk} = -\nu^2 = -(b+1)^{-2}\alpha^2 + O(1)\ (\alpha \to -\infty), \quad \textit{for } k = 0, 1, \ldots, n-2\ .$$

Similarly, the one rogue eigenvalue for $(\Lambda_m, \mathring{B}_m)$ satisfies

$$\mathring{\lambda}_{mm} = -\nu^2 = -\alpha^2 + O(1) \qquad (\alpha \to -\infty).$$

The other eigenvalues in the first band Σ_0^m *satisfy*

$$\mathring{\lambda}_{mk} = -\nu^2 = -(b+1)^{-2}\alpha^2 + O(1) \quad (\alpha \to -\infty), \ \textit{for } k = 0, 1, \ldots, m-1 \ .$$

Proof. In Corollary 12, we showed that the two unconstrained components of the zero set of $D_n(y,z)$ have the asymptotic behavior as $y \to \infty$ in the yz-plane.

$$\begin{aligned} \mathcal{C}_{n,n-1} \ &: \ \alpha z + b\,y - b\,y^{-1} + O(y^{-2}) = 0 \quad (y \to \infty), \\ \mathcal{C}_{nn} \ &: \ \alpha z + y - y^{-1} + O(y^{-2}) = 0 \qquad (y \to \infty). \end{aligned} \tag{5.66}$$

We know that the intersection of the zero set Z_n of D_n with the parametric curve $(y,z) = (c(\lambda), s(\lambda))$ give us the eigenvalues λ of the quantum-tree operator.

In Lemma 15, we proved that as $y \to \infty$, with $\lambda = -\nu^2 < 0$, there exists an asymptotic relation

$$\nu \ = \ -c^{-1}\alpha + O(\alpha^{-1}) \qquad (\alpha \to -\infty),$$

where the parametric curve $(y,z) = (c(\lambda), s(\lambda))$ intersects with curves of this form

$$\alpha z + cy + v_0 + O(y^{-1}) \ = \ 0 \qquad (y \to \infty) \ .$$

Here c is a real number constant. Therefore, the intersection of the parametric curve $(y,z) = (c(\lambda), s(\lambda))$ with the two unconstrained components as shown in equations (5.66) of the zero set of D_n, where $c = b$ and $c = 1$, produce the two rogue eigenvalues that satisfy

$$\begin{aligned} \lambda_{n,n-1} = -\nu^2 = -b^{-2}\alpha^2 + O(1) \quad (\alpha \to -\infty) \\ \lambda_{nn} = -\nu^2 = -\alpha^2 + O(1) \quad (\alpha \to -\infty). \end{aligned}$$

The other eigenvalues, for $k = 0, 1, \ldots, n-2$, are produced by the zero set that are constrained in the slanted lines

$$\alpha z + (b+1)y + (b+1) = 0$$

$$\alpha z + (b+1)y - (b+1) = 0,$$

where in both cases $c = (b+1)$. They thus satisfy

$$\lambda_{nk} = -\nu^2 = -(b+1)^{-2}\alpha^2 + O(1) \quad (\alpha \to -\infty).$$

Similar arguments can be used to show the results for $\mathring{\lambda}_{mk}$, for $k = 0, 1, \ldots, m$. $\square$

So far, we have done all the analysis and proofs that will draw us to the main theorem on the spectrum $\sigma(\Gamma_n, A_n)$ of homogeneous regular quantum tree. Recall that after we illustrated the structure of the homogeneous regular quantum tree and the domain of the Schrödinger operator on the tree, we described how the spectrum of such a tree Γ_n can be reduced by symmetry to the sum of the spectra of $n+1$ linear graphs, with prescribed multiplicities. Following that, we reduce the linear quantum trees to linear combinatorial graphs with the assistance of the transfer matrix that involves two spectral functions $c(\lambda)$ and $s(\lambda)$ depending on potential q. The Robin vertex conditions amount to a homogeneous linear systems with $D_n(\lambda)$ and $\mathring{D}_n(\lambda)$ denoting the determinants of the matrices. The roots of $D_n(\lambda)$ and $\mathring{D}_n(\lambda)$ give the eigenvalues of the linear quantum tree. We find that the functions $D_n(\lambda)$ and $\mathring{D}_n(\lambda)$ are orthogonal polynomials in an appropriately chosen variable because of the three-term recurrence relations they satisfy. We use this connection to orthogonal polynomials to analyze the spectrum of the homogeneous quantum trees in a graphical way.

We separate the roles of the potential q from the Robin prameter α and the branching number b by looking at the parametric curve $(c(\lambda), s(\lambda))$ and the zero level sets Z_n, $\mathring{Z}_n$ independently. We proved that Z_n consists of $n+1$ disjoint curves $\mathcal{C}_{nk}$ with two of them unconstrained when $c(\lambda) = y \to \infty$, and $\mathring{Z}_n$ consists of n disjoint curves $\mathring{\mathcal{C}}_{nk}$ with one of them unconstrained when $c(\lambda) = y \to \infty$. We further presented the exact asymptotics of those unconstrained components as $y \to \infty$. For the parametric curve $\mathcal{S} = ((\lambda), s(\lambda))$, we drew from the literature of their asymptotic behaviors as $\lambda = -\nu^2$ and $\nu^2 \to \infty$. Finally, we looked at the intersections of the Z_n and $\mathring{Z}_n$ with $\mathcal{S}$ to find the spectrum of the homogeneous quantum tree (Γ_n, A_n). The analysis on the intersections tell us the spectral "bands" Σ_k^n and $\mathring{\Sigma}_k^n$ plus the asymptotic behaviors of the rogue eigenvalues as $\alpha \to -\infty$. We summarize the results for the whole spectra of a homogeneous quantum tree (Γ_n, A_n) with branching number b and Robin parameter α in the following theorem.

Theorem 17. *The spectrum $\sigma(\Gamma_n, A_n)$ of the homogeneous regular quantum tree (Γ_n, A_n) with n levels and branching number b is decomposed as*

$$\sigma(\Gamma_n, A_n) = \sigma(\Lambda_n, B_n) \cup \bigcup_{m=1}^{n} \sigma(\Lambda_m, \mathring{B}_m), \tag{5.67}$$

where $\sigma(\Lambda_n, B_n)$ occurs with multiplicity 1 and $\sigma(\Lambda_m, \mathring{B}_m)$ occurs with multiplicity $b^{(n-m)}(b-1)$. Let $\{\lambda_k^*\}_{k=1}^{\infty}$ denote the roots of $s(\lambda)$. Recall that $\lambda_k^* \to \infty$ as $k \to \infty$ and that these do not depend on α or b, but only on $q(x)$.

(i) *$\sigma(\Lambda_n, B_n)$ consists of bands Σ_k^n, $k = 0, 1, 2, \ldots,$ of eigenvalues plus two rogue eigenvalues $\lambda_=^n$ and λ_-^n. For $k \geq 1$, the kth band Σ_k^n contains n eigenvalues λ with*

$$\lambda_k^* \leq \lambda < \lambda_{k+1}^* \qquad (\lambda \in \Sigma_k^n, k \geq 1). \tag{5.68}$$

The band Σ_0^n contains $n-1$ eigenvalues λ such that $\lambda < \mu$ for all $\mu \in \Sigma_1^n$ and

$$\lambda = -(b+1)^{-2}\alpha^2 + O(1) \quad (\alpha \to -\infty) \quad (\lambda \in \Sigma_0^n). \tag{5.69}$$

The rogue eigenvalues satisfy

$$\lambda_=^n = -\alpha^2 + O(1) \qquad (\alpha \to -\infty) \tag{5.70}$$

$$\lambda_-^n = -b^{-2}\alpha^2 + O(1) \qquad (\alpha \to -\infty). \tag{5.71}$$

(ii) *$\sigma(\Lambda_m, \mathring{B}_m)$ consists of bands $\mathring{\Sigma}_k^m$, $k = 0, 1, 2, \ldots,$ of eigenvalues plus one rogue eigenvalue $\lambda_=^m$. For $k \geq 1$, the kth band $\mathring{\Sigma}_k^m$ contains $m-1$ eigenvalues*

λ with

$$\lambda_k^* \leq \lambda < \lambda_{k+1}^* \quad (\lambda \in \mathring{\Sigma}_k^m,\ k \geq 1). \tag{5.72}$$

The band $\mathring{\Sigma}_0^m$ contains $m-1$ eigenvalues λ such that $\lambda < \mu$ for all $\mu \in \mathring{\Sigma}_1^m$ and

$$\lambda = -(b+1)^{-2}\alpha^2 + O(1) \quad (\alpha \to -\infty) \quad (\lambda \in \mathring{\Sigma}_0^m). \tag{5.73}$$

The rogue eigenvalue satisfies

$$\mathring{\lambda}_{=}^m = -\alpha^2 + O(1) \quad (\alpha \to -\infty). \tag{5.74}$$

Proof. The decomposition of the spectrum $\sigma(\Gamma_n, A_n)$ into the sum of the spectrum of linear trees $\sigma(\Lambda_n, B_n)$ and $\sigma(\Lambda_m, \mathring{B}_m)$ with multiplicity 1 and multiplicity $b^{(n-m)}(b-1)$ is discussed in Chapter 3.

The roots λ_k^* of $s(\lambda)$ approaches ∞ as $k \to \infty$. This is proved in Theorem 14. In this same theorem, we also showed that $\sigma(\Lambda_n, B_n)$ consists of bands Σ_k^n, $k = 0, 1, 2, \ldots$, and for $k \geq k_o$, the kth band Σ_k^n contains n eigenvalues λ with

$$\lambda_k^* \leq \lambda < \lambda_{k+1}^* \quad (\lambda \in \Sigma_k^n,\ k \geq 1). \tag{5.75}$$

We also proved in the same manner in this theorem that $\sigma(\Lambda_m, \mathring{B}_m)$ consists of bands $\mathring{\Sigma}_k^m$, $k = 0, 1, 2, \ldots$, of eigenvalues, and for $k \geq \mathring{k}_0$, the kth band $\mathring{\Sigma}_k^m$ contains $m-1$ eigenvalues λ with

$$\lambda_k^* \leq \lambda < \lambda_{k+1}^* \quad (\lambda \in \mathring{\Sigma}_k^m,\ k \geq 1). \tag{5.76}$$

The asymptotics of the eigenvalues in the first bands Σ_0^n and $\mathring{\Sigma}_0^m$, together with the rogue eigenvalues $\lambda_{=}^n$ and λ_{-}^n for $\sigma(\Lambda_n, B_n)$, and the one rogue eigenvalue $\mathring{\lambda}_{=}^m$ for $\sigma(\Lambda_m, \mathring{B}_m)$ as $\alpha \to -\infty$ is proved in Theorem 16. $\square$

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Vita

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