A Discrete and Continuous Dictionary

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Chapter 1

Introduction

There are several results in the fields of second order linear ordinary differential equations and second order linear finite difference equations that seem to be the same 'in spirit'. One such example is Liouville's Formula, which we can apply to second order ordinary differential equations to obtain a first order linear differential equation for the determinant of a fundamental matrix solution:

Theorem 1.1 (Liouville's Formula for Second Order ODEs)**.** *Suppose that we have the arbitrary second order ordinary differential equation:*

$$y'' + p(x)y' + q(x)y = 0,$$

which can be written as the first order system:

$$\begin{pmatrix} y \\ y' \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -q(x) & -p(x) \end{pmatrix} \begin{pmatrix} y \\ y' \end{pmatrix} \iff \dot{u} = B(x)u,\ u \in \mathbb{R}^2.$$

Suppose that the fundamental matrix solution to this system is:

$$\Phi(x) := \begin{pmatrix} y_1(x) & y_2(x) \\ y_1'(x) & y_2'(x) \end{pmatrix}.$$

The Wronskian $W(x)$ is defined as the determinant of $\Phi(x)$. Liouville's Formula states that:

$$\det \Phi(x) = \det \Phi(0) e^{\int_0^x \operatorname{tr} B(s) ds} \text{ or } W(x) = W(0)e^{-\int_0^x p(s)ds}.$$

The discrete analogue states that the determinant of a fundamental set of solutions to a second order linear finite difference equation also obeys a first order finite difference rule:

Theorem 1.2 (Discrete Analogue of Liouville's Formula; Akhiezer [1])**.** *Suppose that we have the arbitrary second order finite difference equation:*

$$b_{k-1}y_{k-1} + a_k y_k + b_k y_{k+1} = \lambda y_k \ (k = 1, 2, 3, ...),$$

which can be written as the first order system:

$$\begin{pmatrix} y_k \\ y_{k-1} \end{pmatrix}_{+1} = \begin{pmatrix} \frac{\lambda - a_k}{b_k} & -\frac{b_{k-1}}{b_k} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} y_k \\ y_{k-1} \end{pmatrix}.$$

Suppose that the fundamental set of solutions to this system is:

$$\Psi(\lambda) = \begin{pmatrix} P_k(\lambda) & Q_k(\lambda) \\ P_{k-1}(\lambda) & Q_{k-1}(\lambda) \end{pmatrix},$$

where $P_k(\lambda)$ and $Q_k(\lambda)$ are orthogonal polynomial solutions of the first and second kind, defined by appropriate initial conditions. The solutions satisfy the following relation:

$$P_{k-1}(\lambda)Q_k(\lambda) - P_k(\lambda)Q_{k-1}(\lambda) = \frac{1}{b_{k-1}} \ (k = 1, 2, 3, ...).$$

In this essay, we aim to uncover more of the connections between the discrete and continuous fields through an investigation of second order symmetric ordinary differential equations and second order symmetric finite difference equations.

We begin by approaching the continuous field. In Chapter 2, we introduce a class of second order periodic ordinary differential equations called the Hill's equation. One area of interest when considering these equations is the conditions required to obtain stable solutions, which typically means periodic or quasiperiodic solutions. We obtain a canonical form for solutions to these equations by applying Liouville's Formula and Floquet's Theorem. We then extend this analysis by considering the Hill's equation as an eigenequation. In particular, we apply Hill equation theory, such as the Oscillation Theorem and the Hill's discriminant, to determine eigenvalues such that the solutions will be stable.

We then shift our focus to the discrete field. In Chapter 3, we introduce the theory of second order symmetric finite difference equations from a classical moment problem perspective. We begin with an overview of functionals, infinite Jacobi matrices and orthogonal polynomials. We then use these infinite Jacobi matrices to generate symmetric second order finite difference equations with orthogonal polynomial solutions. We also delve into some interesting properties of these orthogonal polynomials, observing potential similarities to significant results in the theory of linear differential equations. We conclude the chapter by classifying Jacobi matrices as being of type C or type D, which will have significance in Chapter 4.

In Chapter 4, we aim to bring the discrete and continuous fields together. We first determine how the Hill's equation can be converted to a second order symmetric finite difference equation by applying Fourier series and transforms. We also generate polynomials of the bi-infinite Jacobi matrix, in an attempt to determine whether or not the theory of Chapter 3 still holds. On the other hand, we explore how the infinite Jacobi matrix associated with a certain second order symmetric finite difference equation generates an isometric operator. This allows us to treat our system of orthogonal polynomials as generalised Fourier coefficients of solutions to the periodic ordinary differential equation. We conclude by working through a few examples, such as special differential equations known to have a system of orthogonal polynomials that satisfy (not necessarily symmetric) finite difference equations.

Chapter 2

Periodic Ordinary Differential Equations

2.1 The Hill's Equation

A key element to understanding the connections between the discrete and continuous fields comes from the symmetry of the associated differential operator. Hence, we begin our investigation by studying a class of homogeneous, linear, second order differential equations with periodic coefficients, known as the Hill's equation.

The Hill's equation can be used to describe motions of the moon, since the moon's motion can be viewed as a harmonic oscillator in a periodic gravitational field. This model equation arises in many areas of applied mathematics where the stability of periodic motions is an issue. Another example is the stability analysis of small oscillations of a pendulum whose length varies with time (Chicone [5]). We define the Hill's equation as an equation of the form:

$$y'' + V(x)y = 0,$$

where $V(x+T) = V(x)$, in other words, the potential $V(x)$ is a T-periodic function. In addition, we define the Hill's equation in the standard form as:

$$y'' + [\lambda + V(x)]y = 0,$$

where $V(x)$ is a T-periodic function assumed to be bounded on $\mathbb{R}$, and λ is a parameter. One of the main areas of interest for this equation is the determination of eigenvalues λ for which the solutions are stable. We will also be interested in the monodromy matrix.

Definition 2.1 (Stable and Unstable Solutions)**.** *A solution to the Hill's equation is stable if it is bounded for all $x \in \mathbb{R}$. A solution to the Hill's equation is unstable if it is unbounded.*

Definition 2.2 (Monodromy Matrix)**.** *A monodromy matrix is the principal fundamental matrix of a periodic system of ordinary differential equations, evaluated at an integer multiple of the period of the coefficients of the system. In other words, if the principal fundamental matrix solution is $\Phi(x)$, then the monodromy matrix is $\Phi(nT)$ for $n \in \mathbb{Z}$.*

2.2 Stability Analysis of the Hill's Equation

2.2.1 Floquet's Theorem

Floquet's Theorem can be applied to give results concerning the stability of solutions. In this section, we introduce and prove Floquet's Theorem. Let us begin by defining:

$$u := \begin{pmatrix} y \\ y' \end{pmatrix}.$$

Then the Hill's equation is equivalent to the first order system:

$$\begin{pmatrix} y \\ y' \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -V(x) & 0 \end{pmatrix} \begin{pmatrix} y \\ y' \end{pmatrix} \Longleftrightarrow \dot{u} = A(x)u,\ u \in \mathbb{R}^2, \tag{2.3}$$

where $x \mapsto A(x)$ is a T-periodic continuous matrix-valued function. Floquet's Theorem provides a canonical form for the fundamental matrix of linear systems of the form (2.3). This result will be used to show that there is a periodic time-dependent change of co-ordinates that transforms (2.3) into a homogeneous linear system with constant coefficients. We will use Theorem 2.4 and Theorem 2.5 to prove Floquet's Theorem:

Theorem 2.4 (Chicone [5]). *If $x \mapsto A(x)$ is continuous on the interval $x \in (\alpha, \beta)$ and if $x_0 \in (\alpha, \beta)$, where possibly $\alpha = -\infty$ or $\beta = \infty$, then the solution of the initial value problem $\dot{u} = A(x)u$, $u(x_0) = u_0$, is defined on the open interval (α, β).*

Theorem 2.5 (Chicone [5]). *If C is a non-singular $n \times n$ matrix, then there is an $n \times n$ matrix B (possibly complex) such that $e^B = C$. If C is a non-singular real $n \times n$ matrix, then there is a real $n \times n$ matrix B such that $e^B = C^2$.*

Theorem 2.6 (Floquet's Theorem). *If $\Phi(x)$ is a fundamental matrix solution of the T-periodic system (2.3), then for all $x \in \mathbb{R}$:*

$$\Phi(x + T) = \Phi(x)\Phi^{-1}(0)\Phi(T).$$

In addition, there is a matrix B (possibly complex) such that:

$$e^{TB} = \Phi^{-1}(0)\Phi(T)$$

and a T-periodic matrix function $x \mapsto P(x)$ (possibly complex) such that:

$$\Phi(x) = P(x)e^{xB} \text{ for all } x \in \mathbb{R}.$$

Also, there is a real matrix R and a real $2T$-periodic matrix function $x \mapsto Q(x)$ such that:

$$\Phi(x) = Q(x)e^{xR} \text{ for all } x \in \mathbb{R}.$$

Proof of Floquet's Theorem. Since the function $x \mapsto A(x)$ is periodic, then it is defined for all $x \in \mathbb{R}$. By Theorem 2.4, it follows that all solutions of the system are defined for $x \in \mathbb{R}$.

If $\Psi(x) := \Phi(x+T)$, then $\Psi(x)$ is a matrix solution, since:

$$\dot{\Psi}(x) = \dot{\Phi}(x+T) = A(x+T)\Phi(x+T) = A(x)\Psi(x).$$

We define:

$$C := \Phi^{-1}(0)\Phi(T) = \Phi^{-1}(0)\Psi(0),$$

and note that C is non-singular (invertible). The matrix function $x \mapsto \Phi(x)C$ is a matrix solution of the linear system with initial value $\Phi(0)C = \Psi(0)$. By the uniqueness of solutions, we have $\Phi(x)C = \Psi(x)$ for all $x \in \mathbb{R}$. In particular, we have that:

$$\begin{aligned}\Psi(x) = \Phi(x+T) = \Phi(x)C = \Phi(x)\Phi^{-1}(0)\Phi(T)\\ \Psi(x+T) = \Phi(x+2T) = \Phi(x+T)C = \Phi(x)C^2\end{aligned}$$

By Theorem 2.5, there exists a matrix B such that $e^{TB} = C$. Also, there is a real matrix R such that $e^{2TR} = C^2$. If we define $P(x) = \Phi(x)e^{-xB}$ and $Q(x) = \Phi(x)e^{-xR}$, then:

$$\begin{aligned}P(x+T) = \Phi(x+T)e^{-xB}e^{-TB} = \Phi(x)Ce^{-xB}e^{-TB} = \Phi(x)e^{-xB} = P(x)\\ Q(x+2T) = \Phi(x+2T)e^{-xR}e^{-2TR} = \Phi(x)C^2e^{-xR}e^{-2TR} = \Phi(x)e^{-xR} = Q(x)\end{aligned}$$

Thus, we have $P(x+T) = P(x)$ and $Q(x+2T) = Q(x)$, and:

$$\Phi(x) = P(x)e^{xB} = Q(x)e^{xR} \text{ for all } x \in \mathbb{R}. \qquad \square$$

2.2.2 Application to the Hill's Equation

We now perform a stability analysis on the Hill's equation, written as the first order system (2.3). We suppose that the principal fundamental matrix is given by $\Phi(x)$, with initial conditions uniquely defined such that the solutions will be continuously differentiable and normalised:

$$\Phi(x) = \begin{pmatrix} y_1(x) & y_2(x) \\ y_1'(x) & y_2'(x) \end{pmatrix}, \; \Phi(0) = \begin{pmatrix} y_1(0) & y_2(0) \\ y_1'(0) & y_2'(0) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{2.7}$$

The first step in the stability analysis is an application of Liouville's Formula (Theorem 1.1) to $\Phi(x)$ of (2.3) at $x = 0$. This gives:

$$\det\Phi(x) = \det\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} e^0 = 1.$$

Definition 2.8 (Characteristic Multiplier)**.** *A characteristic multiplier is an eigenvalue of the monodromy matrix $\Phi(T)$.*

By Liouville's Formula, the product of the characteristic multipliers is also equal to one. Let us denote these eigenvalues as λ_1 and λ_2. They are the roots of the characteristic equation:

$$\begin{aligned}&\lambda^2 - (\mathrm{tr}\Phi(T))\lambda + \det\Phi(T) = 0\\ &\implies \lambda^2 - 2\phi\lambda + 1 = 0 \text{ (by setting } 2\phi := \mathrm{tr}\Phi(T))\\ &\implies \lambda = \phi \pm \sqrt{\phi^2 - 1}\end{aligned}$$

As the second step in our stability analysis, we apply Floquet's Theorem to determine the nature of the solutions to (2.3). This leads us to the following theorem:

Theorem 2.9 (Stability of Solutions; Magnus and Winkler [9]). *Suppose that $\Phi(x)$ is the fundamental matrix solution of (2.3). The general solution is stable if and only if* $\left|\mathrm{tr}\Phi(T)\right| < 2$, *or* $\mathrm{tr}\Phi(T) = \pm 2$ *and* $\Phi(T) = I$*, where I is the identity matrix.*

Proof. By applying Floquet's Theorem to the Hill's equation, we have the following results:

If $\phi > 1$, then λ_1 and λ_2 are distinct, positive real numbers such that $\lambda_1\lambda_2 = 1$. Then we may assume that $0 < \lambda_1 < 1 < \lambda_2$ with $\lambda_1 = \frac{1}{\lambda_2}$ and there is a real number $\mu > 0$ such that $\lambda_1 = e^{T\mu}$ and $\lambda_2 = e^{-T\mu}$. There is a fundamental set of solutions of the form:

$$e^{-\mu x}p_1(x),\ e^{\mu x}p_2(x),$$

where the real functions p_1, p_2 are T-periodic. In this case, all solutions will be unbounded, hence the general solution is unstable.

If $\phi < -1$, then λ_1 and λ_2 are real and negative. Since $\lambda_1\lambda_2 = 1$, we may assume that $\lambda_1 < -1 < \lambda_2 < 0$ with $\lambda_1 = \frac{1}{\lambda_2}$. Thus, there is a real number $\mu > 0$ such that $\lambda_1^2 = e^{2T\mu}$ and $\lambda_2^2 = e^{-2T\mu}$. There is a fundamental set of solutions of the form:

$$e^{-\mu x}q_1(x),\ e^{\mu x}q_2(x),$$

where the real functions q_1, q_2 are $2T$-periodic. In this case, all solutions will be unbounded, hence the general solution is unstable.

If $-1 < \phi < 1$, then λ_1 and λ_2 are complex conjugates with non-zero imaginary part. Since $\lambda_1\overline{\lambda_1} = 1$, then $|\lambda_1| = 1$ and therefore both characteristic multipliers lie on the unit circle in the complex plane. Say that λ_1 lies in the upper half plane for example. Then there is a real number α such that $0 < \alpha T < \pi$ and $e^{i\alpha T} = \lambda_1$. There is a solution of the form $e^{i\alpha x}(r(x) + is(x))$ with r and s both T-periodic functions, hence we can write the fundamental set of solutions as:

$$r(x)\cos\alpha x - s(x)\sin\alpha x,\ r(x)\sin\alpha x + s(x)\cos\alpha x.$$

In this case, the solutions are stable. Also, the solutions are periodic if and only if there are relatively prime positive integers m, n such that $\frac{2\pi m}{\alpha} = nT$. If such integers exist, all solutions have period nT. If not, then all solutions are quasiperiodic.

If $\phi = 1$, then $\lambda_1 = \lambda_2 = 1$ and the nature of the solutions will depend on the canonical form of $\Phi(T)$. If $\Phi(T)$ is the identity, then $e^0 = \Phi(T)$ and there is a Floquet normal form $\Phi(x) = P(x)$ where $P(x)$ is T-periodic and invertible. Thus, there is a fundamental set of periodic solutions and the general solution is stable. If $\Phi(T)$ is not the identity, then there is a non-singular matrix C such that:

$$C\Phi(T)C^{-1} = I + N = e^N,$$

where $N \neq 0$ is nilpotent. Thus, $\Phi(x)$ has a Floquet normal form $\Phi(x) = P(x)e^{xB}$ where $B := C^{-1}(\frac{1}{T}N)C$. Because:

$$e^{xB} = C^{-1}(1 + \frac{x}{T}N)C,$$

the function $x \mapsto e^{xB}$ is linearly growing and unbounded, creating an unstable general solution.

If $\phi = -1$, then the situation is similar to the previous case, except $\Phi(x) = Q(x)e^{xB}$, where $Q(x)$ is a $2T$-periodic function. $\square$

2.2.3 The Hill's Equation with Symmetric Potential

We have the following result for the Hill's equation with symmetric potential:

Theorem 2.10 (Magnus and Winkler [9]). *Let $y_1(x)$ and $y_2(x)$ be the normalised solutions of (2.3), where $V(x+T) = V(x) = V(-x)$. Then the following relations hold:*

$$y_1(T) = 2y_1\Big(\frac{T}{2}\Big)y_2'\Big(\frac{T}{2}\Big) - 1 = 1 + 2y_1'\Big(\frac{T}{2}\Big)y_2\Big(\frac{T}{2}\Big) \tag{2.11}$$

$$y_2(T) = 2y_2\Big(\frac{T}{2}\Big)y_2'\Big(\frac{T}{2}\Big) \tag{2.12}$$

$$y_1'(T) = 2y_1\Big(\frac{T}{2}\Big)y_1'\Big(\frac{T}{2}\Big) \tag{2.13}$$

$$y_2'(T) = y_1(T) \tag{2.14}$$

In all cases, $y_1(x) = y_1(-x)$ and $y_2(x) = -y_2(-x)$. Whenever a non-trivial T- or $2T$-periodic solution exists, there also exists such a solution which is either odd or even. Therefore, the periodic solutions are multiples of $y_1(x)$ or $y_2(x)$, unless all solutions are T- or $2T$-periodic.

Proof. If $V(x)$ is even and $y(x)$ is a solution of (2.3), then $y(-x)$ is also a solution because:

$$y''(x)+V(x)y(x) = y''(x)+V(-x)y(x) = y''(-x)+V(x)y(-x) = y''(-x)+V(-x)y(-x) = 0.$$

Since the initial conditions for $y_1(-x)$ and $y_1(x)$ coincide, and similarly for $y_2(x)$ and $-y_2(-x)$, then $y_1(x)$ is even and $y_2(x)$ is odd. By Floquet's Theorem, we can write solutions of the form:

$$\begin{aligned}
\begin{pmatrix} y_1(x+T) & y_2(x+T) \\ y_1'(x+T) & y_2'(x+T) \end{pmatrix} &= \frac{1}{\det\Phi(0)} \begin{pmatrix} y_1(x) & y_2(x) \\ y_1'(x) & y_2'(x) \end{pmatrix} \begin{pmatrix} y_2'(0) & -y_2(0) \\ -y_1'(0) & y_1(0) \end{pmatrix} \begin{pmatrix} y_1(T) & y_2(T) \\ y_1'(T) & y_2'(T) \end{pmatrix} \\
&= \begin{pmatrix} y_1(x) & y_2(x) \\ y_1'(x) & y_2'(x) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} y_1(T) & y_2(T) \\ y_1'(T) & y_2'(T) \end{pmatrix} \\
&= \begin{pmatrix} y_1(x)y_1(T) + y_2(x)y_1'(T) & y_1(x)y_2(T) + y_2(x)y_2'(T) \\ y_1'(x)y_1(T) + y_2'(x)y_1'(T) & y_1'(x)y_2(T) + y_2'(x)y_2'(T) \end{pmatrix}
\end{aligned}$$

Hence, we have the system of equations:

$$\begin{aligned} y_1(x+T) &= y_1(x)y_1(T) + y_2(x)y_1'(T) \\ y_2(x+T) &= y_1(x)y_2(T) + y_2(x)y_2'(T) \end{aligned} \tag{2.15}$$

Substituting $x = -\frac{T}{2}$ into (2.15), and recalling that $y_1(x)$ is even while $y_2(x)$ is odd gives:

$$y_1\Big(\frac{T}{2}\Big) = y_1\Big(\frac{-T}{2}\Big)y_1(T) + y_2\Big(\frac{-T}{2}\Big)y_1'(T) = y_1\Big(\frac{T}{2}\Big)y_1(T) - y_2\Big(\frac{T}{2}\Big)y_1'(T) \tag{2.16}$$

$$y_2\Big(\frac{T}{2}\Big) = y_1\Big(\frac{-T}{2}\Big)y_2(T) + y_2\Big(\frac{-T}{2}\Big)y_2'(T) = y_1\Big(\frac{T}{2}\Big)y_2(T) - y_2\Big(\frac{T}{2}\Big)y_2'(T) \tag{2.17}$$

Since $y_1'(x)$ is odd and $y_2'(x)$ is even, differentiating the equations in system (2.15) with respect to x and substituting $x = -\frac{T}{2}$ gives:

$$y_1'\left(\frac{T}{2}\right) = y_1'\left(\frac{-T}{2}\right)y_1(T) + y_2'\left(\frac{-T}{2}\right)y_1'(T) = -y_1'\left(\frac{T}{2}\right)y_1(T) + y_2'\left(\frac{T}{2}\right)y_1'(T) \tag{2.18}$$

$$y_2'\left(\frac{T}{2}\right) = y_1'\left(\frac{-T}{2}\right)y_2(T) + y_2'\left(\frac{-T}{2}\right)y_2'(T) = -y_1'\left(\frac{T}{2}\right)y_2(T) + y_2'\left(\frac{T}{2}\right)y_2'(T) \tag{2.19}$$

Hence, from equations (2.16), (2.17), (2.18) and (2.19) we obtain the following system:

$$\begin{aligned}
y_1\left(\frac{T}{2}\right) &= y_1\left(\frac{T}{2}\right)y_1(T) - y_2\left(\frac{T}{2}\right)y_1'(T)\\
y_1'\left(\frac{T}{2}\right) &= -y_1'\left(\frac{T}{2}\right)y_1(T) + y_2'\left(\frac{T}{2}\right)y_1'(T)\\
y_2\left(\frac{T}{2}\right) &= y_1\left(\frac{T}{2}\right)y_2(T) - y_2\left(\frac{T}{2}\right)y_2'(T)\\
y_2'\left(\frac{T}{2}\right) &= -y_1'\left(\frac{T}{2}\right)y_2(T) + y_2'\left(\frac{T}{2}\right)y_2'(T)
\end{aligned}$$

We also recall that, from the application of Liouville's Formula, the Wronskian equals one:

$$y_1\left(\frac{T}{2}\right)y_2'\left(\frac{T}{2}\right) - y_1'\left(\frac{T}{2}\right)y_2\left(\frac{T}{2}\right) = 1.$$

Putting these results together gives statements (2.11), (2.12), (2.13) and (2.14) of Theorem 2.10. In addition, if $y(x)$ is of period T or $2T$, the functions:

$$\begin{aligned}
u(x) &= y(x) + y(-x)\\
v(x) &= y(x) - y(-x)
\end{aligned}$$

have the same property. Since $u(x)$ is even and $v(x)$ is odd, and they cannot be trivial unless $y(x) = 0$, then the last statement of Theorem 2.10 holds. □

Example 2.20. In order to see Theorem 2.9 and Theorem 2.10 in practice, we numerically compute solutions to the homogeneous Hill's equation with potential $V(x) = \cos(2x)$. Since

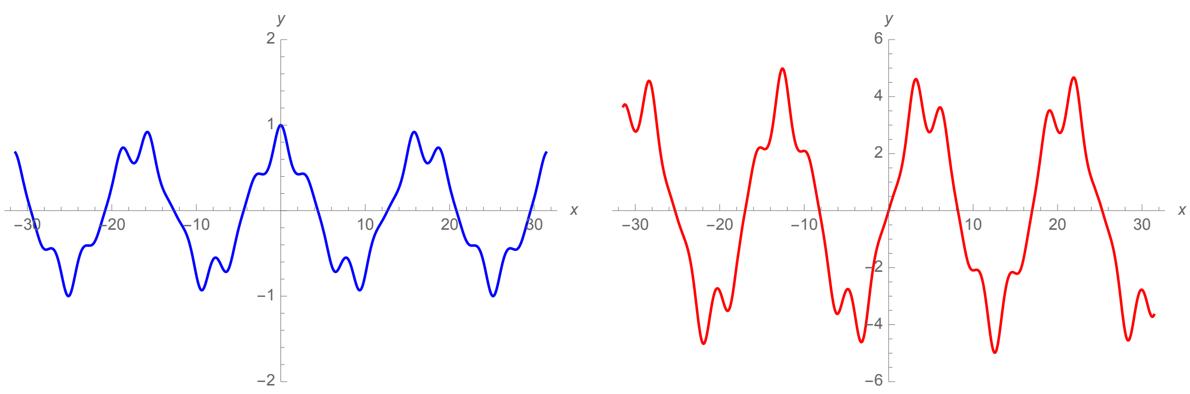

Figure 2.20.1: Solutions $y_1(x)$ and $y_2(x)$ to the equation $y'' + \cos(2x)y = 0$.

we have bounded (and thus stable) solutions for all $x \in \mathbb{R}$, by Theorem 2.9 we expect to see that $\left|\mathrm{tr}\Phi(T)\right| < 2$, or both $\mathrm{tr}\Phi(T) = \pm 2$ and $\Phi(T) = I$ hold. We verify this by numerically computing the trace of the monodromy matrix:

$$\left|y_1(\pi) + y_2'(\pi)\right| \approx 0.772651 < 2.$$

Since $\cos(2x)$ is an even function, we also verify that Theorem 2.10 holds. As expected, we can see that $y_1(x)$ is an even function and $y_2(x)$ is an odd function. In addition, we have:

$$y_1(\pi) = 1 + 2y_1'\left(\frac{\pi}{2}\right)y_2\left(\frac{\pi}{2}\right) \approx 0.386326 \qquad y_2(\pi) = 2y_2\left(\frac{\pi}{2}\right)y_2'\left(\frac{\pi}{2}\right) \approx 4.59748$$
$$y_1'(\pi) = 2y_1\left(\frac{\pi}{2}\right)y_1'\left(\frac{\pi}{2}\right) \approx -0.185048 \qquad y_2'(\pi) = y_1(\pi) \approx 0.386326$$

2.3 Eigenvalues and Intervals of Stability

2.3.1 The Oscillation Theorem

As mentioned in Section 2.1, one area of interest when considering the Hill's equation is the determination of eigenvalues λ for which solutions are stable. In this section, we introduce a theorem that allows us to determine these eigenvalues. We can consider the Hill's equation in the standard form as a first order system:

$$\begin{pmatrix} y \\ y' \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -\lambda - V(x) & 0 \end{pmatrix} \begin{pmatrix} y \\ y' \end{pmatrix} \Longleftrightarrow \dot{u} = A(x;\lambda)u,\ u \in \mathbb{R}^2, \tag{2.21}$$

where $x \mapsto A(x;\lambda)$ is a T-periodic continuous matrix-valued function and λ is a parameter. Theorem 2.22 allows us to define intervals of stability for the solutions of (2.21).

Theorem 2.22 (Oscillation Theorem; Magnus and Winkler [9]). *For every differential equation* (2.21)*, there exist two monotonically increasing infinite sequences of real numbers:*

$$\lambda_0, \lambda_1, \lambda_2, \lambda_3, \ldots \text{ and } \lambda_1', \lambda_2', \lambda_3', \lambda_4', \ldots$$

such that (2.21) *has a solution of period:*

- T *if and only if* $\lambda = \lambda_n$, $n \geq 0$.
- $2T$ *if and only if* $\lambda = \lambda_n'$, $n \geq 1$.

Then, λ_n *and* λ_n' *satisfy the inequalities:*

$$\lambda_0 < \lambda_1' \leq \lambda_2' < \lambda_1 \leq \lambda_2 < \lambda_3' \leq \lambda_4' < \lambda_3 \leq \lambda_4 < \ldots \tag{2.23}$$

where $(\lambda_n)^{-1} \to 0$ *and* $(\lambda_n')^{-1} \to 0$ *as* $n \to \infty$*. The solutions of* (2.21) *are stable in the intervals:*

$$(\lambda_0, \lambda_1'), (\lambda_2', \lambda_1), (\lambda_2, \lambda_3'), (\lambda_4', \lambda_3), \ldots$$

The solutions at the endpoints of these intervals are generally unstable. This is always true for $\lambda = \lambda_0$*. The solutions are also unstable for* $\lambda \notin \mathbb{R}$*.*

The solutions are stable for:

- $\lambda = \lambda_{2n+1}$ *or* $\lambda = \lambda_{2n+2}$*, if and only if* $\lambda_{2n+1} = \lambda_{2n+2}$.
- $\lambda = \lambda'_{2n+1}$ *or* $\lambda = \lambda'_{2n+2}$*, if and only if* $\lambda'_{2n+1} = \lambda'_{2n+2}$.

The λ_n *are the roots of* $\Delta(\lambda) = 2$*, and the* λ'_n *are the roots of* $\Delta(\lambda) = -2$*, where:*

$$\Delta(\lambda) = y_1(T;\lambda) + y_2'(T;\lambda) =: \mathrm{tr}\Phi(T;\lambda).$$

2.3.2 Results Concerning Eigenvalues of the Hill's Equation

We have the following result concerning the eigenvalues of the Hill's equation with a potential $V(x)$ that is T-periodic, complex and such that $V(-x) = \overline{V(x)}$:

Theorem 2.24. *If* $V(x)$ *is a complex* T*-periodic function,* $V(-x) = \overline{V(x)}$ *and there exists a solution to* (2.21)*, then* $\lambda \in \mathbb{R}$.

Proof. We define the operator $L := \partial_{xx} + V(x)$ on the space of T-periodic functions f, g, and use the following inner product:

$$\langle f, g\rangle = \int_0^T f\bar{g}dx.$$

For f and g, which are periodic or quasiperiodic solutions to (2.21), we have:

$$\begin{aligned}
\langle f, Lg\rangle &= \int_0^T (f\bar{g}'' + f\overline{V(x)g})dx \\
&= [f\bar{g}']_0^T - [f'\bar{g}]_0^T + \int_0^T f''\bar{g}dx + \int_0^T f\overline{V(x)}\bar{g}dx \\
&= \int_0^T f''\bar{g}dx + \int_0^T fV(-x)\bar{g}dx \text{ (by periodicity of } f, g) \\
&= \int_0^T f''\bar{g}dx + \int_{-T}^0 fV(x)\bar{g}dx \\
&= \int_0^T f''\bar{g}dx + \int_0^T fV(x)\bar{g}dx \text{ (by periodicity of potential)} \\
&= \langle Lf, g\rangle
\end{aligned}$$

$$\implies \int_0^T f\bar{\lambda}\bar{g}dx = \int_0^T \lambda f\bar{g}dx \implies \lambda = \bar{\lambda} \implies \lambda \in \mathbb{R}.$$

□

We also have the following result concerning the eigenvalues of monodromy operators:

Theorem 2.25 (Chicone [5])**.** *All monodromy operators have the same eigenvalues. That is, the spectrum of* $\Phi(T)$ *is equal to the spectrum of* $\Phi(nT)$ *for* $n \in \mathbb{Z}$.

Proof. Consider the principal fundamental matrix $\Phi(x)$ at $x = 0$. Then:

$$\Psi(x) := \Phi(x)\Psi(0) \implies \Psi(0) = \Phi(0)\Psi(0) \implies \Phi(0) = \Phi^{-1}(0) = 1.$$

Let us consider the monodromy operator $\mathcal{M}$ given by $v \mapsto \Psi(T+\tau)\Psi^{-1}(\tau)v$. It follows that:

$$\begin{aligned}
\Psi(T+\tau)\Psi^{-1}(\tau) &= \Phi(T+\tau)\Psi(0)\Psi^{-1}(0)\Phi^{-1}(\tau) \\
&= \Phi(T+\tau)\Phi^{-1}(\tau) \\
&= \Phi(T)\Phi^{-1}(0)\Phi(\tau)\Phi^{-1}(\tau) \text{ (by Floquet's Theorem)} \\
&= \Phi(T)\Phi(\tau)\Phi^{-1}(\tau) \ (\because \Phi^{-1}(0) = 1) \\
&= \Phi(T)
\end{aligned}$$

Hence, the eigenvalues of the operator $\Phi(T)$ are the same as the eigenvalues of the monodromy operator $\mathcal{M}$, implying that all monodromy operators have the same eigenvalues. □

Example 2.26. We attempt to visually verify the claim given in Theorem 2.25. From the Oscillation Theorem (Theorem 2.22), we recall that eigenvalues can be determined by solving for λ, when $\Delta(\lambda) = \pm 2$. In this example, we consider the Hill's equation in the standard form with potential $V(x) = 2\cos(x)$, otherwise known as a form of the Mathieu equation:

$$y'' + [\lambda + 2\cos(x)]y = 0.$$

The monodromy operators occur at period $nT := 2n\pi$, for $n \in \mathbb{Z}$. Hence, we plot the function:

$$\Delta^*(\lambda) := y_1(2n\pi) + y_2'(2n\pi),$$

for various monodromy operators. We also include the horizontal lines $\Delta(\lambda) = \pm 2$ in red, to emphasise eigenvalues and the intervals of stability.

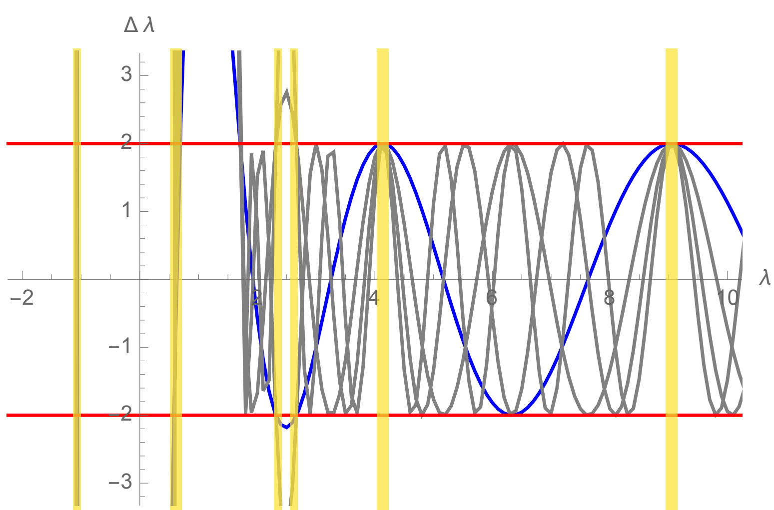

Figure 2.26.1: Monodromy operators for $n = 1, ..., 10$. The blue curve represents the canonical monodromy operator (where $n = 1$). The yellow bars represent approximate ranges for some of the eigenvalues.

While it is difficult to see in Figure 2.26.1, the claim of Theorem 2.25 seems to hold in that the monodromy operators have the same eigenvalues. In other words, the monodromy operators intersect with the functions $\Delta(\lambda) = \pm 2$ for the same values of λ.

2.3.3 The Hill's Discriminant

In the previous section, we introduced the function:

$$\Delta(\lambda) := \mathrm{tr}\Phi(T;\lambda) = y_1(T;\lambda) + y_2'(T;\lambda), \tag{2.27}$$

which allows us to discriminate between values of λ for which the solutions of (2.21) are stable or unstable. For this reason, we establish the following definition:

Definition 2.28 (Hill's Discriminant)**.** *The function* (2.27) *is called the discriminant of the Hill's equation* (2.21)*, or the Hill's discriminant for short.*

Example 2.29. We aim to understand how the Hill's discriminant and the Oscillation Theorem (Theorem 2.22) can be used to determine information considering the periodic spectrum of the Hill's equation operator. As in Example 2.26, we once again consider the Mathieu equation as an example:

$$y'' + [\lambda + 2\cos(x)]y = 0.$$

To begin with, we plot the Hill's discriminant $\Delta(\lambda)$ as a function of λ. We include the horizontal lines $\Delta(\lambda) = \pm 2$ to highlight the intervals of stability:

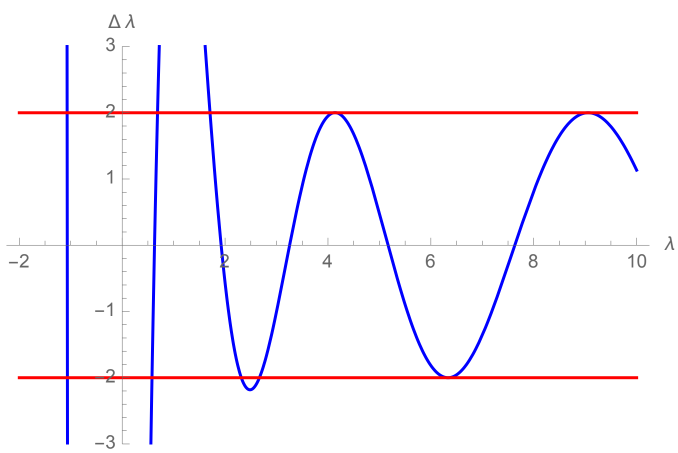

Figure 2.29.1: Hill's discriminant for $y'' + [\lambda + 2\cos(x)]y = 0$.

According to Theorem 2.22, we can numerically compute the eigenvalues by solving for λ when $\Delta(\lambda) = \pm 2$. These eigenvalues will also form the endpoints of the intervals of stability. Some examples of the eigenvalues numerically computed for this equation are (to the nearest 0.05):

$$\lambda \approx 0.7,\ 1.75,\ 2.2,\ 2.75,\ 4.25,\ 4.5,\ 6.2,\ 6.45, \ldots$$

While it is difficult to observe in Figure 2.29.1, this suggests that there are actually an infinite number of (fairly small) intervals of stability for this equation as $\lambda \to \infty$. We also remark that the spectrum of this Hill differential operator seems to be simple, in that the eigenvalues are all distinct. However, without the appropriate tools, we cannot conclude this for certain, since there appear to be an infinite number of eigenvalues. We will introduce such tools for determining information about the spectrum in the following chapters.

Chapter 3

Symmetric Finite Difference Equations

3.1 The Moment Problem Approach

In Chapter 2, we focused on a class of second order periodic ordinary differential equations known as the Hill's equation, and uncovered results concerning the stability of solutions. We now turn our attention to the orthogonal polynomial solutions of symmetric second order finite difference equations, introducing them from a classical moment problem perspective. Stieltjes writes, in Chapter 4 of his "Investigations on Continued Fractions" (Stieltjes [11]):

We shall call the "moment problem" the following problem: to find a positive mass distribution on a straight line $[0, \infty)$*, given the moments of order* k $(k = 0, 1, 2, 3, ...)$.

To give a distribution of positive mass on $[0, \infty)$ means to give a non-decreasing function $\sigma(u)$ $(u \geq 0)$ such that for any $\alpha \geq 0$ and $\beta > \alpha$, the increase of $\sigma(\beta) - \sigma(\alpha)$ represents the mass in the interval $[\alpha, \beta)$. The total mass on the line $[0, \infty)$ may therefore be written as:

$$\lim_{\beta \to \infty} [\sigma(\beta) - \sigma(0)] = \int_0^\infty d\sigma(u).$$

Assuming that we can call the following integral "a generalised moment of order k":

$$\int_0^\infty u^k d\sigma(u),$$

we can define a solution $\sigma(u)$ of the moment problem to be:

$$s_k = \int_0^\infty u^k d\sigma(u) \ (k = 0, 1, 2, ...). \tag{3.1}$$

In particular, we will introduce the concepts of positive sequences, functionals and infinite Jacobi matrices as well as their associated orthogonal polynomials, which are derived from Hankel matrices. These concepts will then allow us to link the limiting behaviour of these polynomials to the spectrum of the associated Jacobi operator.

3.2 Infinite Jacobi Matrices and their Polynomials

3.2.1 Basic Concepts

Definition 3.2 (Positive Sequence)**.** *A positive sequence is an infinite sequence of real numbers $\{s_k\}_0^\infty$ such that all quadratic (Hankel) forms:*

$$\sum_{i,k=0}^{m} s_{i+k}x_i x_k \ (m = 0, 1, 2, ...)$$

are positive definite. We note that the positive definite property of the sequence $\{s_k\}_0^\infty$ is equivalent to the claim that the determinant of the associated Hankel matrix is positive:

$$D_k = \begin{vmatrix} s_0 & s_1 & \dots & s_k \\ s_1 & s_2 & \dots & s_{k+1} \\ \dots & \dots & \dots & \dots \\ s_k & s_{k+1} & \dots & s_{2k} \end{vmatrix} > 0 \ (k = 0, 1, 2, ...).$$

Definition 3.3 (Infinite Jacobi Matrix)**.** *An infinite Jacobi matrix is a matrix of the form:*

$$\begin{pmatrix} a_0 & b_0 & 0 & 0 & 0 & \dots \\ b_0 & a_1 & b_1 & 0 & 0 & \dots \\ 0 & b_1 & a_2 & b_2 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \tag{3.4}$$

such that $a_k \in \mathbb{R}$ and $b_k > 0$ for all $k \in \mathbb{N}$.

Definition 3.5 (Functional)**.** *A functional is a real-valued function on a vector space. For any sequence of numbers $\{s_k\}_0^\infty$, we can define a functional $\mathcal{S}$ in the space of polynomials by:*

$$\mathcal{S}\{R(\lambda)\} = p_0 s_0 + p_1 s_1 + ... + p_n s_n, \text{ where } R(\lambda) = p_0 + p_1\lambda + ... + p_n\lambda^n.$$

This functional is additive and homogeneous, in other words, it is linear in the algebraic sense.

3.2.2 Construction of Associated Polynomials

One can typically construct the polynomials associated with an infinite Jacobi matrix by applying the Gram-Schmidt process to the sequence of functions λ^k $(k = 0, 1, 2, ...)$, taking:

$$\langle \lambda^i, \lambda^k \rangle = s_{i+k}$$

as the scalar product, where s_{i+k} is some element of a positive sequence $\{s_m\}_0^\infty$. This process will result in polynomials that are orthogonal and normalised with respect to a certain sequence of polynomials. In this section, we introduce an alternative definition for an arbitrary orthonormal polynomial that uses determinants of Hankel matrices. This will allow us to take a moment problem approach towards the construction of the associated Jacobi operator.

Definition 3.6 (Orthonormal Polynomials)**.** *Suppose that we have the positive sequence* $\{s_k\}_0^\infty$. *The polynomials* $P_n(\lambda)$ $(n = 0, 1, 2, ...)$ *are orthogonal and normalised (orthonormal) with respect to the sequence:*

$$P_0(\lambda), P_1(\lambda), P_2(\lambda), ...$$

if the sequence has the following properties:

1. $P_n(\lambda)$ *is a polynomial of exact degree* n *and its leading coefficient is positive.*

2. *The following orthogonality relation holds:*

$$\mathcal{S}\{P_m(\lambda)P_n(\lambda)\} = \delta_{mn} = \begin{cases} 0 & (m \neq n) \\ 1 & (m = n) \end{cases}$$

We now introduce an explicit expression for these orthonormal polynomials in terms of determinants. We begin with the initial condition $P_0(\lambda) = 1$. Recalling the determinantal definition of a positive sequence (Definition 3.2), we can define an arbitrary polynomial by:

$$\begin{aligned} P_n(\lambda) &= \frac{1}{\sqrt{D_{n-1}D_n}} \begin{vmatrix} s_0 & s_1 & ... & s_n \\ s_1 & s_2 & ... & s_{n+1} \\ ... & ... & ... & ... \\ s_{n-1} & s_n & ... & s_{2n-1} \\ 1 & \lambda & ... & \lambda^n \end{vmatrix} \quad (n = 1, 2, 3, ...) \\ &= \frac{1}{\sqrt{D_{n-1}D_n}}[D_{n-1}\lambda^n + R_{n-1}(\lambda)], \text{ where } R_{n-1}(\lambda) \text{ is some polynomial of degree } n-1 \\ &= \sqrt{\frac{D_{n-1}}{D_n}}\lambda^n + R_{n-1}(\lambda) \end{aligned}$$

To show that these polynomials $P_n(\lambda)$ satisfy the orthogonality relation, we verify that:

$$\mathcal{S}\{P_n(\lambda)\lambda^m\} = \begin{cases} 0 & (m = 0, 1, 2, ..., n-1) \\ \sqrt{\frac{D_n}{D_{n-1}}} & (m = n) \end{cases} \tag{3.7}$$

This is because if (3.7) is true, then substituting the definition of $P_m(\lambda)$ gives:

$$\begin{aligned} \mathcal{S}\{P_m(\lambda)P_n(\lambda)\} &= \mathcal{S}\Big\{P_n(\lambda)\Big[\sqrt{\frac{D_{m-1}}{D_m}}\lambda^m + R_{m-1}(\lambda)\Big]\Big\} \\ &= \mathcal{S}\Big\{P_n(\lambda)\sqrt{\frac{D_{m-1}}{D_m}}\lambda^m\Big\} + \mathcal{S}\{P_n(\lambda)R_{m-1}(\lambda)\} \text{ (by linearity of } \mathcal{S}) \\ &= \sqrt{\frac{D_{m-1}}{D_m}}\mathcal{S}\{P_n(\lambda)\lambda^m\} + \mathcal{S}\{P_n(\lambda)R_{m-1}(\lambda)\} \text{ (by linearity of } \mathcal{S}) \end{aligned}$$

Since $n = m - 1 \implies n \neq m$, then by orthogonality it follows that $\mathcal{S}\{P_n(\lambda)R_{m-1}(\lambda)\} = 0$. Hence, this actually leaves us with the relation:

$$\mathcal{S}\{P_m(\lambda)P_n(\lambda)\} = \sqrt{\frac{D_{m-1}}{D_m}}\mathcal{S}\{P_n(\lambda)\lambda^m\}.$$

To begin the proof of (3.7), we first note the identity:

$$P_n(\lambda)\lambda^m = \frac{1}{\sqrt{D_{n-1}D_n}} \begin{vmatrix} s_0 & s_1 & \dots & s_n \\ s_1 & s_2 & \dots & s_{n+1} \\ \dots & \dots & \dots & \dots \\ s_{n-1} & s_n & \dots & s_{2n-1} \\ \lambda^m & \lambda^{m+1} & \dots & \lambda^{m+n} \end{vmatrix} \ (n = 1, 2, 3, \dots).$$

Applying the functional $\mathcal{S}$ to both sides results in the following:

- When $m = 0, 1, 2, \dots, n-1$, the final row of the matrix coincides with one of the previous rows. Hence, by row reduction the determinant will be equal to zero, giving the result:

$$\mathcal{S}\{P_n(\lambda)\lambda^m\} = 0 \ (m = 0, 1, 2, \dots, n-1).$$

- When $m = n$, we have:

$$P_n(\lambda)\lambda^m = \frac{1}{\sqrt{D_{n-1}D_n}} \begin{vmatrix} s_0 & s_1 & \dots & s_n \\ s_1 & s_2 & \dots & s_{n+1} \\ \dots & \dots & \dots & \dots \\ s_{n-1} & s_n & \dots & s_{2n-1} \\ \lambda^n & \lambda^{n+1} & \dots & \lambda^{2n} \end{vmatrix} \ (n = 1, 2, 3, \dots)$$

$$\implies \mathcal{S}\{P_n(\lambda)\lambda^m\} = \frac{D_n}{\sqrt{D_{n-1}D_n}} = \sqrt{\frac{D_n}{D_{n-1}}} \ (m = n). \quad \square$$

3.2.3 Derivation of Second Order Finite Difference Equations

We now use these orthonormal polynomials to define a second order finite difference equation, such that the polynomials will be solutions to the difference equation. To begin with, any arbitrary polynomial may be expanded in terms of the polynomials $P_k(\lambda)$. To show this, we write polynomials in the form:

$$\lambda P_k(\lambda) = a_{k,k+1}P_{k+1}(\lambda) + a_{k,k}P_k(\lambda) + a_{k,k-1}P_{k-1}(\lambda) + \dots, \tag{3.8}$$

where $a_{k,k+1}$, $a_{k,k}$, $a_{k,k-1}$, ... can be seen as being entries of an infinite matrix. Comparison of the leading coefficients gives:

$$LHS = \lambda P_k(\lambda) = \sqrt{\frac{D_{k-1}}{D_k}}\lambda^{k+1}$$

$$RHS = a_{k,k+1}\sqrt{\frac{D_k}{D_{k+1}}}\lambda^{k+1} + a_{k,k}\sqrt{\frac{D_{k-1}}{D_k}}\lambda^k + a_{k,k-1}\sqrt{\frac{D_{k-2}}{D_{k-1}}}\lambda^{k-1} + \dots$$

$$\implies \sqrt{\frac{D_{k-1}}{D_k}} = a_{k,k+1}\sqrt{\frac{D_k}{D_{k+1}}} \implies a_{k,k+1} = \frac{\sqrt{D_{k-1}D_{k+1}}}{D_k}$$

Multiplying both sides of (3.8) by $P_i(\lambda)$ $(i = 0, 1, ..., k)$ and applying the functional $\mathcal{S}$ to the relation:

$$\lambda P_k(\lambda) = a_{k,k+1} P_{k+1}(\lambda) + a_{k,k} P_k(\lambda) + a_{k,k-1} P_{k-1}(\lambda)$$

gives the following results:

$$a_{k,i} = 0 \ (i = 0, 1, 2, ..., k-2),\ a_{k,k-1} = \mathcal{S}\{\lambda P_k(\lambda) P_{k-1}(\lambda)\} \text{ and } a_{k,k} = \mathcal{S}\{\lambda P_k(\lambda) P_k(\lambda)\}.$$

Substituting $\lambda P_{k-1}(\lambda) = a_{k-1,k} P_k(\lambda) + R_{k-1}(\lambda)$ into the expression for $a_{k,k-1}$ then gives:

$$\lambda P_{k-1}(\lambda) P_k(\lambda) = [a_{k-1,k} P_k(\lambda) + R_{k-1}(\lambda)] P_k(\lambda) = a_{k-1,k} P_{2k}(\lambda) + R_{2k-1}(\lambda)$$
$$\implies \mathcal{S}\{\lambda P_{k-1}(\lambda) P_k(\lambda)\} = a_{k-1,k} s_{2k} + ...$$

Since $\mathcal{S}\{\lambda P_k(\lambda) P_{k-1}(\lambda)\} = \mathcal{S}\{\lambda P_{k-1}(\lambda) P_k(\lambda)\}$, we also have $a_{k,k-1} = a_{k-1,k}$. Therefore the expansion (3.8) takes the form:

$$\lambda P_k(\lambda) = b_{k-1} P_{k-1}(\lambda) + a_k P_k(\lambda) + b_k P_{k+1}(\lambda) \ (k = 0, 1, 2, ...),$$

where we define:

$$b_{-1} = 0,\ a_k = a_{k,k} = \mathcal{S}\{\lambda P_k(\lambda) P_k(\lambda)\} \text{ and } b_k = a_{k,k+1} = \frac{\sqrt{D_{k-1} D_{k+1}}}{D_k}.$$

Hence, we have obtained the symmetric second order finite difference equation:

$$b_{k-1} y_{k-1} + a_k y_k + b_k y_{k+1} = \lambda y_k \ (k = 1, 2, 3, ...), \text{ with initial condition } (a_0 - \lambda) y_0 + b_0 y_1 = 0.$$

Example 3.9. We can generate a system of orthonormal polynomials using appropriate initial conditions and the recursion relation above. As an example, let us take $a_k = -k^2$, $b_k = 1$, giving us the following second order finite difference equation:

$$y_{k-1} - k^2 y_k + y_{k+1} = \lambda y_k. \tag{3.10}$$

While setting these values may not seem to be very meaningful at the moment, we will see that this finite difference equation describes the Jacobi matrix of the Mathieu equation. As we will see in Section 4.4.2, collecting the coefficients of the real Fourier series allows us to write (3.10) as an infinite matrix of the form:

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & ... \\ 2 & -1 & 1 & 0 & 0 & 0 & ... \\ 0 & 1 & -4 & 1 & 0 & 0 & ... \\ 0 & 0 & 1 & -9 & 1 & 0 & ... \\ 0 & 0 & 0 & 1 & -16 & 1 & ... \\ ... & ... & ... & ... & ... & ... & ... \end{pmatrix} \tag{3.11}$$

While (3.11) is technically not a Jacobi matrix due to its lack of symmetry, in Section 4.5.2 we will see that we can actually symmetrise the matrix, if required. Nonetheless, we can compute orthogonal polynomials of the first and second kind, based on the initial conditions:

$$\begin{aligned} P_0(\lambda) &= 1 & Q_0(\lambda) &= 0 \\ P_1(\lambda) &:= \frac{\lambda - a_0}{b_0} = \lambda & Q_1(\lambda) &:= \frac{1}{b_0} = 1 \end{aligned}$$

The initial conditions for $Q_n(\lambda)$ were chosen such that the system of polynomials would be linearly independent and normalised. Substituting the initial conditions and computing the polynomials for the finite difference equations (3.11) gives the following system:

$$\begin{array}{ll}
P_0(\lambda) = 1 & Q_0(\lambda) = 0 \\
P_1(\lambda) = \lambda & Q_1(\lambda) = 1 \\
P_2(\lambda) = \lambda^2 + \lambda - 2 & Q_2(\lambda) = \lambda + 1 \\
P_3(\lambda) = \lambda^3 + 5\lambda^2 + \lambda - 8 & Q_3(\lambda) = \lambda^2 + 5\lambda + 3 \\
P_4(\lambda) = \lambda^4 + 14\lambda^3 + 45\lambda^2 - 70 & Q_4(\lambda) = \lambda^3 + 14\lambda^2 + 47\lambda + 26 \\
\quad ... & \quad ...
\end{array}$$

3.3 Properties of the Associated Polynomials

3.3.1 Polynomials of the First and Second Kind

The finite difference equation:

$$b_{k-1}y_{k-1} + a_k y_k + b_k y_{k+1} = \lambda y_k \ (k = 1, 2, 3, ...) \tag{3.12}$$

has two linearly independent solutions. In Example 3.9, we saw that we can define them by:

Polynomials of the first kind	Polynomials of the second kind
$P_k(\lambda)$ is of exact degree k	$Q_k(\lambda)$ is of exact degree $k-1$
$P_0(\lambda) = 1,\ P_1(\lambda) = \dfrac{\lambda - a_0}{b_0}$	$Q_0(\lambda) = 0,\ Q_1(\lambda) = \dfrac{1}{b_0}$

The following identity provides a link between the polynomials of first and second kind:

$$Q_k(\lambda) = \mathcal{S}\Big\{\frac{P_k(\lambda) - P_k(u)}{\lambda - u}\Big\}.$$

We verify this by using the determinantal definition of $P_k(\lambda)$:

$$\begin{aligned}
\frac{P_k(\lambda) - P_k(u)}{\lambda - u} &= \frac{\sqrt{\frac{D_{k-1}}{D_k}}\lambda^k + R_{k-1}(\lambda) - \sqrt{\frac{D_{k-1}}{D_k}}u^k - R_{k-1}(u)}{\lambda - u} \\
&= \frac{\sqrt{\frac{D_{k-1}}{D_k}}(\lambda^k - u^k) + R_{k-1}(\lambda) - R_{k-1}(u)}{\lambda - u} \\
&= \sqrt{\frac{D_{k-1}}{D_k}}(\lambda^{k-1} + \lambda^{k-2}u + ... + \lambda u^{k-2} + u^{k-1}) + \frac{R_{k-1}(\lambda) - R_{k-1}(u)}{\lambda - u}
\end{aligned}$$

$\Longrightarrow \mathcal{S}\Big\{\dfrac{P_k(\lambda) - P_k(u)}{\lambda - u}\Big\} = Q_k(\lambda)$, where $Q_k(\lambda)$ is a polynomial of exact degree $k-1$.

We can obtain the following results (Theorem 3.13 and Theorem 3.15), which are analogous to significant results in the theory of linear differential equations:

Theorem 3.13 (Discrete Analogue of Liouville's Formula; Akhiezer [1]). *Suppose that $P_k(\lambda)$ and $Q_k(\lambda)$ are orthogonal polynomials of the first and second kind satisfying* (3.12). *Then:*

$$P_{k-1}(\lambda)Q_k(\lambda) - P_k(\lambda)Q_{k-1}(\lambda) = \frac{1}{b_{k-1}} \; (k = 1, 2, 3, ...). \tag{3.14}$$

Proof. We prove (3.14) by induction on k. When $k = 1$, we have:

$$LHS = P_0(\lambda)Q_1(\lambda) - P_1(\lambda)Q_0(\lambda) = 1 \cdot \frac{1}{b_0} - \frac{\lambda - a_0}{b_0} \cdot 0 = \frac{1}{b_0} = RHS.$$

We assume the induction hypothesis (3.14). Using the fact that $P_k(\lambda)$ and $Q_k(\lambda)$ are solutions to the recurrence relation (3.12), we have:

$$\begin{aligned}
&P_k(\lambda)Q_{k+1}(\lambda) - P_{k+1}(\lambda)Q_k(\lambda)\\
&= P_k(\lambda)\Big[\frac{(\lambda - a_k)Q_k(\lambda) - b_{k-1}Q_{k-1}(\lambda)}{b_k}\Big] - Q_k(\lambda)\Big[\frac{(\lambda - a_k)P_k(\lambda) - b_{k-1}P_{k-1}(\lambda)}{b_k}\Big]\\
&= \frac{P_{k-1}(\lambda)Q_k(\lambda)b_{k-1} - P_k(\lambda)Q_{k-1}(\lambda)b_{k-1}}{b_k} = \frac{b_{k-1} \cdot \frac{1}{b_{k-1}}}{b_k} = \frac{1}{b_k}
\end{aligned}$$

□

Theorem 3.15 (Discrete Analogue of Green's Formula; Akhiezer [1]). *Suppose that y_k and z_k are solutions of* (3.12)*, with parameters λ and μ respectively. Then:*

$$b_{n-1}(y_{n-1}z_n - y_nz_{n-1}) - b_{m-1}(y_{m-1}z_m - y_mz_{m-1}) = (\mu - \lambda)\sum_{k=m}^{n-1} y_kz_k. \tag{3.16}$$

Proof. We have the following system of equations:

$$\begin{cases} b_{k-1}y_{k-1} + a_ky_k + b_ky_{k+1} &= \lambda y_k \\ b_{k-1}z_{k-1} + a_kz_k + b_kz_{k+1} &= \mu z_k \end{cases} \Longrightarrow \begin{cases} b_{k-1}y_{k-1}z_k + a_ky_kz_k + b_ky_{k+1}z_k &= \lambda y_kz_k \\ b_{k-1}y_kz_{k-1} + a_ky_kz_k + b_ky_kz_{k+1} &= \mu y_kz_k \end{cases}$$

It follows that:

$$\begin{aligned}
(\mu - \lambda)y_kz_k &= b_{k-1}(y_kz_{k-1} - y_{k-1}z_k) + b_k(y_kz_{k+1} - y_{k+1}z_k)\\
\Longrightarrow \; (\mu - \lambda)\sum_{k=m}^{n-1} y_kz_k &= \sum_{k=m}^{n-1}[b_{k-1}(y_kz_{k-1} - y_{k-1}z_k) + b_k(y_kz_{k+1} - y_{k+1}z_k)]
\end{aligned}$$

Since we have a telescoping sum, this gives the result (3.16). □

Substituting $y_k = P_k(\lambda)$, $z_k = P_k(\mu)$ and $m = 1$ in (3.16) gives the so-called:

$$\text{Christoffel-Darboux formula } (\mu - \lambda)\sum_{k=0}^{n-1} P_k(\lambda)P_k(\mu) = b_{n-1}[P_{n-1}(\lambda)P_n(\mu) - P_n(\lambda)P_{n-1}(\mu)].$$

In addition, if we substitute $m = 1, \mu = \bar{\lambda}$ ($\mathrm{Im}(\lambda) \neq 0$), $y_k = \omega P_k(\lambda) + Q_k(\lambda)$ and $z_k = \bar{y}_k$ in (3.16), where ω is a complex parameter, we obtain the following equation which plays a role in Theorem 3.20:

$$\sum_{k=0}^{n-1}\big|\omega P_k(\lambda) + Q_k(\lambda)\big|^2 - \frac{\omega - \bar{\omega}}{\lambda - \bar{\lambda}} = b_{n-1}\big|\omega P_{n-1}(\lambda) + Q_{n-1}(\lambda)\big|^2 \frac{\mathrm{Im}\Big(\frac{\omega P_n(\lambda) + Q_n(\lambda)}{\omega P_{n-1}(\lambda) + Q_{n-1}(\lambda)}\Big)}{\mathrm{Im}(\lambda)}.$$

3.3.2 Discrete Analogue of the Oscillation Theorem

We prove a theorem that can be viewed as a discrete analogue of the Oscillation Theorem (Theorem 2.22). To begin with, we introduce the notion of a quasiorthogonal polynomial:

Definition 3.17 (Quasiorthogonal Polynomial)**.** *A quasiorthogonal polynomial of degree n is a polynomial of the form:*

$$\alpha P_n(\lambda) - \beta P_{n-1}(\lambda) = P_n(\lambda; \alpha, \beta),$$

where α and β are parameters that do not become zero simultaneously. If $\alpha \neq 0$, we have:

$$P_n(\lambda; \alpha, \beta) = \alpha P_n\Big(\lambda; \frac{\beta}{\alpha}\Big), \text{ where } P_n(\lambda; \tau) = P_n(\lambda) - \tau P_{n-1}(\lambda).$$

The following orthogonality relation also holds:

$$\mathcal{S}\{P_n(\lambda; \alpha, \beta)\lambda^k\} = 0 \ (k = 0, 1, 2, ..., n-2).$$

Theorem 3.18 (Akhiezer [1])**.** *The following statements hold:*

1. *All the zeroes of a real quasiorthogonal polynomial are real and simple.*
2. *Any two zeroes of $P_n(\lambda)$ are separated by a zero of $P_{n-1}(\lambda)$, and vice versa.*
3. *The zeroes of $Q_n(\lambda)$ are real and simple and any two of them are separated by a zero of $P_n(\lambda)$, and vice versa.*

Proof. Proving each statement, we have:

1. Assume that the real quasiorthogonal polynomial $P_n(\lambda; \tau)$ only changes sign at the following points on the real axis: $\lambda_1 < \lambda_2 < ... < \lambda_m$. Then, the polynomial:

   $$R(\lambda) = P_n(\lambda; \tau)(\lambda - \lambda_1)(\lambda - \lambda_2)...(\lambda - \lambda_m) \neq 0$$

   is non-negative on the real axis and therefore $\mathcal{S}\{R(\lambda)\} > 0$. However, this contradicts the orthogonality relation if $m \leq n-2$. Therefore, $m \geq n-1$, in other words, $P_n(\lambda; \tau)$ has at least $n-1$ simple real zeroes. Hence, all its zeroes are real and simple.

2. From the Christoffel-Darboux formula, as $\mu \to \lambda$ we have:

   $$\sum_{k=0}^{n-1} [P_k(\lambda)]^2 = b_{n-1}[P_{n-1}(\lambda)P_n'(\lambda) - P_n(\lambda)P_{n-1}'(\lambda)].$$

   If λ_1 and λ_2 are two neighbouring zeroes of the polynomial $P_n(\lambda)$, then the numbers $P_n'(\lambda_1)$ and $P_n'(\lambda_2)$ are of different sign, and we have:

   $$b_{n-1}P_{n-1}(\lambda_1)P_n'(\lambda_1) = \sum_{k=0}^{n-1}[P_k(\lambda_1)]^2 > 0 \text{ and } b_{n-1}P_{n-1}(\lambda_2)P_n'(\lambda_2) = \sum_{k=0}^{n-1}[P_k(\lambda_2)]^2 > 0.$$

   Therefore, $P_{n-1}(\lambda_1)$ and $P_{n-1}(\lambda_2)$ are of different signs and hence the statement follows.

3. The first half of the statement can be proven analogously to Statement 1. The second half of the statement follows from the discrete analogue of Liouville's Formula, since the proof will hold for (3.14) if we replace $P_n'(\lambda)$ with $Q_n(\lambda)$ in our proof of Statement 2. $\square$

3.3.3 Circular Contours

The system of orthonormal polynomials exhibits some interesting behaviour as their degrees increase. Using quasiorthogonal polynomials, we can define the following functions:

$$\omega_n(\lambda;\tau) = -\frac{Q_n(\lambda) - \tau Q_{n-1}(\lambda)}{P_n(\lambda) - \tau P_{n-1}(\lambda)} =: -\frac{Q_n(\lambda;\tau)}{P_n(\lambda;\tau)}, \tag{3.19}$$

which are functions of the complex variable λ, the real parameter τ (where $-\infty < \tau \leq \infty$) and the index n. From the definition of this function, we have:

$$\omega_n(\lambda;\infty) = -\lim_{\tau\to\infty} \frac{Q_n(\lambda) - \tau Q_{n-1}(\lambda)}{P_n(\lambda) - \tau P_{n-1}(\lambda)} = -\lim_{\tau\to\infty} \frac{\frac{Q_n(\lambda)}{\tau} - Q_{n-1}(\lambda)}{\frac{P_n(\lambda)}{\tau} - P_{n-1}(\lambda)} = -\frac{Q_{n-1}(\lambda)}{P_{n-1}(\lambda)} = \omega_{n-1}(\lambda;0).$$

In other words, there exists a point at which the functions ω_n and ω_{n-1} touch. Since by the discrete analogue of Liouville's Formula, we have $P_{k-1}(\lambda)Q_k(\lambda) - P_k(\lambda)Q_{k-1}(\lambda) \neq 0$, then $\omega_n(\lambda;\tau)$ is a Möbius transformation describing a circular contour. The behaviour of these contours is described by Theorem 3.20 and Corollary 3.21:

Theorem 3.20 (Akhiezer [1]). *Let λ be fixed in the half-plane* $\mathrm{Im}(\lambda) > 0$ (or $\mathrm{Im}(\lambda) < 0$) and let τ vary along the whole real axis. Then $\omega = \omega_n(\lambda;\tau)$ describes a circular contour $K_n(\lambda)$ in the half-plane, with:

$$\text{Centre:} \quad -\frac{Q_n(\lambda)\overline{P_{n-1}(\lambda)} - Q_{n-1}(\lambda)\overline{P_n(\lambda)}}{P_n(\lambda)\overline{P_{n-1}(\lambda)} - P_{n-1}(\lambda)\overline{P_n(\lambda)}}, \text{ Radius: } \frac{1}{\left|\lambda - \bar{\lambda}\right|} \frac{1}{\sum_{k=0}^{n-1}\left|P_k(\lambda)\right|^2}.$$

In addition, the equation of the circle $K_n(\lambda)$ may be written in the form:

$$\frac{\omega - \bar{\omega}}{\lambda - \bar{\lambda}} - \sum_{k=0}^{n-1}\left|\omega P_k(\lambda) + Q_k(\lambda)\right|^2 = 0.$$

Corollary 3.21. *$K_{n+1}(\lambda) \subseteq K_n(\lambda)$ for all $n \in \mathbb{N}$.*

Proof. If a point ω lies on the circle $K_{n+1}(\lambda)$, then we have:

$$\frac{\omega - \bar{\omega}}{\lambda - \bar{\lambda}} - \sum_{k=0}^{n}\left|\omega P_k(\lambda) + Q_k(\lambda)\right|^2 = 0 \implies \frac{\omega - \bar{\omega}}{\lambda - \bar{\lambda}} - \sum_{k=0}^{n-1}\left|\omega P_k(\lambda) + Q_k(\lambda)\right|^2 \geq 0,$$

and thus the point ω lies within $K_n(\lambda)$ or on its circumference. The existence of a common point on the circumferences $K_{n+1}(\lambda)$ and $K_n(\lambda)$ follows from $\omega_n(\lambda;\infty) = \omega_{n-1}(\lambda;0)$. □

In summary, it seems that there are two significant properties of our sequence $K_n(\lambda)$; for all $n \in \mathbb{N}$, the circle $K_{n+1}(\lambda)$ lies entirely within the circle $K_n(\lambda)$, and the circumferences of these circles touch. Therefore, there would be two possible options for the sequence; we can have either a limiting point or a limiting circle. Hence, we establish the following definition:

Definition 3.22 (Matrix of Type C or D; Akhiezer [1]). *We say that:*

- *An infinite Jacobi matrix is called a matrix of type C for the case of a limiting circle.*

- *An infinite Jacobi matrix is called a matrix of type D for the case of a limiting point.*

The significance of these cases will be discussed in Chapter 4. The following theorem tells us that the classification of infinite Jacobi matrices is invariant with respect to the choice of λ:

Theorem 3.23 (Invariance of Circular Contours; Akhiezer [1])**.** *Let $K_\infty(\lambda)$ represent the (infinite) sequence of circular contours for an infinite Jacobi matrix. If $K_\infty(\lambda)$ is a circle for some non-real λ, then $K_\infty(\lambda)$ will be a circle for any non-real λ. Furthermore, if the series $\sum_{k=0}^{\infty} \left|P_k(\lambda)\right|^2$ converges at any non-real point λ, then it converges uniformly in every finite part of the complex λ-plane.*

Example 3.24. In Example 3.9, we generated a system of orthogonal polynomials for the infinite matrix (3.11). We now determine its classification. To begin with, we substitute the orthogonal polynomials for $n = 1, ..., 5$ into the function $\omega_n(\lambda; \tau)$ (Figure 3.24.1). Since pairs of circular contours share a common point, $\omega_n(\lambda; \infty) = \omega_{n-1}(\lambda; 0)$ is satisfied by these functions. Corollary 3.21 is also satisfied since the contours lie entirely inside one another as $n \to \infty$.

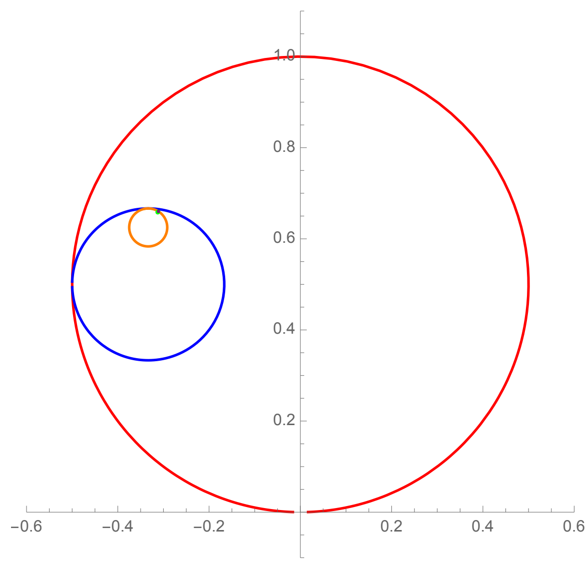

Figure 3.24.1: Circular contours $n = 1, ..., 5$ for the infinite matrix (3.11).

We can visually observe a limiting point as $n \to \infty$. We numerically verify this by checking:

$$\sum_{k=0}^{\infty} \left|P_k(\lambda)\right|^2 \text{ diverges.}$$

The link between the divergence of this series and the classification of infinite Jacobi matrices will be explained in Section 4.3.3. We have the following result for the partial sum:

$$\sum_{k=0}^{20} \left|P_k(i)\right|^2 \approx -4.400 \times 10^{34} - 1.638 \times 10^{34} i \implies \left| \sum_{k=0}^{20} \left|P_k(i)\right|^2 \right| \approx 4.695 \times 10^{34},$$

implying that the series evaluated at $\lambda = i$ diverges. Since Theorem 3.23 tells us that the classification of infinite Jacobi matrices is invariant with respect to λ, we conclude that (3.11) is a matrix of type D by Definition 3.22.

Chapter 4

Connections Between the Discrete and Continuous Fields

4.1 Observations

Intuitively, there seems to be a close connection between second order symmetric finite difference equations and second order symmetric ordinary differential equations. This connection becomes apparent if we take some arbitrary second order symmetric finite difference operator:

$$\begin{aligned} \tau : \ell(\mathbb{Z}) &\mapsto \ell(\mathbb{Z}) \\ f(n) &\mapsto b(n-1)f(n-1) + a(n)f(n) + b(n)f(n+1) \end{aligned}$$

Suppose that we define the finite difference operators, $(\partial f)(n) = f(n+1) - f(n)$ and its "adjoint" $(\partial^* f)(n) = f(n-1) - f(n)$. Then we can rewrite τ as:

$$(\tau f)(n) = -(\partial^*(b\partial f))(n) + (b(n-1) + a(n) + b(n))f(n),$$

because:

$$\begin{aligned} RHS &= -[b(n-1)(f(n) - f(n-1)) - b(n)(f(n+1) - f(n))] + [b(n-1) + a(n) + b(n)]f(n) \\ &= -[b(n-1)f(n) - b(n-1)f(n-1) - b(n)f(n+1) + b(n)f(n)] + [b(n-1) + a(n) + b(n)]f(n) \\ &= b(n-1)f(n-1) + b(n)f(n+1) + a(n)f(n) = (\tau f)(n) = LHS \end{aligned}$$

We recall Leibniz's rule for differentiation under the integral sign:

Theorem 4.1 (Leibniz Rule; Flanders [6]). *For an integral of the form:*

$$\int_{a(x)}^{b(x)} f(x,t)dt,$$

where $-\infty < a(x), b(x) < \infty$*, the derivative of this integral is expressible as:*

$$\frac{d}{dx}\Big(\int_{a(x)}^{b(x)} f(x,t)dt\Big) = f(x, b(x)) \cdot \frac{d}{dx}b(x) - f(x, a(x)) \cdot \frac{d}{dx}a(x) + \int_{a(x)}^{b(x)} \frac{\partial}{\partial x} f(x,t)dt.$$

Since the concept of integration in the calculus sense does not apply to the discrete field, ∂ and ∂^* do not satisfy the Leibniz rule and hence are not derivatives. However, the expression for $(\tau f)(n)$ resembles the Sturm-Liouville form for second order linear differential equations:

$$\frac{d}{dx}\left[p(x)\frac{dy}{dx}\right] + q(x)y = -\lambda w(x)y.$$

There are also several other similarities between differentials, integrals and their discrete counterpart differences and sums. Some of these similarities include the product rules (discrete analogues for the product rule in differentiation):

$$(\partial fg)(n) = f(n)(\partial g)(n) + g(n+1)(\partial f)(n)$$
$$(\partial^* fg)(n) = f(n)(\partial^* g)(n) + g(n-1)(\partial^* f)(n)$$

and the summation by parts formula, otherwise known as the Abel transform (a discrete analogue of integration by parts for continuous variables):

$$\sum_{j=m}^{n} g(j)(\partial f)(j) = g(n)f(n+1) - g(m-1)f(m) + \sum_{j=m}^{n}(\partial^* g)(j)f(j).$$

In this chapter, we aim to understand how we can translate continuous results to discrete results and vice versa. We also aim to gain some insight into the spectral information that we can uncover by making such a transformation.

4.2 Discretising the Hill's Equation

4.2.1 The Hill's Determinant

We begin to investigate the notion of translating a continuous result to a discrete one by introducing the Hill's determinant. We will use the following notation to write the determinant of a matrix:

$$\left\|a_{n,m}\right\|_k^l,$$

where n (row number) and m (column number) vary over all integers from k to l. We are particularly interested in the cases where $k = -\infty$ and $l = \infty$ (a bi-infinite matrix), or where $k = 0$ and $l = \infty$ (an infinite matrix). We also say that the infinite determinants:

$$\left\|a_{n,m}\right\|_0^\infty, \left\|a_{n,m}\right\|_{-\infty}^\infty \text{ exist or converge if the limits } \lim_{l\to\infty}\left\|a_{n,m}\right\|_0^l, \lim_{l\to\infty}\left\|a_{n,m}\right\|_{-l}^l \text{ exist.}$$

The value of the limit is called the value of the determinant, and if the determinant is finite, then we say that it is of Hill's type. More formally, we can use the following definition:

Definition 4.2 (Determinant of Hill's Type)**.** *A determinant is of Hill's type if it satisfies:*

$$\sum_{n,m}\left|a_{n,m} - \delta_{n,m}\right| < \infty, \tag{4.3}$$

where $\delta_{n,m}$ is the Kronecker delta, in other words $\delta_{n,m} = 1$ for $n = m$ and $\delta_{n,m} = 0$ otherwise. The sum (4.3) *is taken over all values of n and m.*

In 1877, George William Hill began to use infinite determinants to study the orbit of the moon, in particular applying them to improve the accuracy of results obtained for the three-body problem (Brown [4]). In this section, we determine how the Hill's equation operator can be represented as an infinite matrix using the Fourier transform. In the following section, we will uncover the remarkable result that the Hill's discriminant can be expressed in terms of the Hill's determinant. First, we use Lemma 4.4 to prove Theorem 4.5.

Lemma 4.4 (Magnus and Winkler [9]). *Let* $\left\|a_{n,m}\right\|_0^\infty$ *be a determinant of Hill's type. Let:*

$$a'_{n,m} = a_{n,m} \text{ if } n \neq m,\ a'_{n,n} = a_{n,n} \text{ if } \left|a_{n,n}\right| \geq 1,\ a'_{n,n} = 1 \text{ if } \left|a_{n,n}\right| < 1,$$

and let:

$$H = \Big[\prod_{n=0}^{\infty}\Big(\sum_{m=0}^{\infty}\left|a'_{n,m}\right|^2\Big)\Big]^{\frac{1}{2}}.$$

Then it follows that $H < \infty$ and the absolute value of any finite subdeterminant of $\left\|a_{n,m}\right\|_0^\infty$ is at most equal to H.

Theorem 4.5 (Magnus and Winkler [9]). *An infinite determinant of Hill's type converges.*

Proof. It suffices to prove this theorem for the determinant $\left\|a_{n,m}\right\|_0^\infty$. According to Hadamard's inequality concerning determinants, we have the following result:

$$|D|^2 \leq \prod_{n=k}^{l}\Big(\sum_{m=k}^{l}\left|a_{n,m}\right|^2\Big), \text{ where } D = \left\|a_{n,m}\right\|_k^l.$$

We can apply Lemma 4.4 here. We can also expand the determinant $\left\|a_{n,m}\right\|_0^{l+1} = D_{l+1}$ in terms of the elements of the last row and their subdeterminants, which can be reordered by H, defined in Lemma 4.4. The result is $D_{l+1} = a_{l+1,l+1}D_l + \theta_l H$, where $|\theta_l| \leq \varepsilon_{l+1}$. Since $|D_l| \leq H$, then:

$$|D_{l+1} - D_l| \leq H\left|a_{l+1,l+1} - 1\right| + H\varepsilon_{l+1} = H\sum_{m=0}^{\infty}\left|a_{l+1,m} - \delta_{l+1,m}\right|$$

$$\implies \sum_{l=1}^{\infty}|D_{l+1} - D_l| < \infty \text{ and } \lim_{l\to\infty} D_{l+1} = D \text{ exists.} \qquad \square$$

The following theorem allows us to make certain assumptions about our infinite determinant:

Theorem 4.6 (Magnus and Winkler [9]). *Let* $\left\|a_{n,m}\right\|$ *be an infinite determinant of Hill's type, and assume that there exist numbers x_m not all of which vanish such that $|x_m| \leq M$ (M fixed) for all m and $\sum_m a_{n,m}x_m = 0$ for all n. Then:*

$$\left\|a_{n,m}\right\| = 0.$$

Proof. Since the set of subdeterminants of $\left\|a_{n,m}\right\|$ is bounded, it follows that for each n, $\left\|a_{n,m}\right\| x_n = 0$. The inequality (4.3) and the condition $|x_m| \leq M$ also guarantee the absolute convergence of all sums involved, hence proving all statements of the theorem. $\square$

We now show how the Hill's equation operator can be represented as an infinite matrix using Fourier series. We begin by expressing the potential of the Hill's equation as a Fourier series:

$$y'' + \Big(\sum_{n=-\infty}^{\infty} g_n e^{2inx}\Big) y = 0, \tag{4.7}$$

where $\lambda = g_0$. For simplicity, we assume that in this case our potential is π-periodic. By Floquet's Theorem, (4.7) has a non-zero solution of the form:

$$y = e^{i\alpha x} p(x), \tag{4.8}$$

where $p(x)$ is a π-periodic function. If $V(x)$ is sufficiently smooth, for example if $\sum |g_n| < \infty$, then the function y in (4.8) can be expanded in a twice termwise-differentiable Fourier series:

$$y(x) = \sum_{n=-\infty}^{\infty} p_n e^{i(\alpha+2n)x}. \tag{4.9}$$

Hence, we can write the left hand side of (4.7) in the following form, using Cauchy products:

$$\begin{aligned}
y'' + \Big(\sum_{n=-\infty}^{\infty} g_n e^{2inx}\Big) y &= -\sum_{n=-\infty}^{\infty} (\alpha+2n)^2 p_n e^{i(\alpha+2n)x} + \Big(\sum_{n=-\infty}^{\infty} g_n e^{2inx}\Big)\Big(\sum_{n=-\infty}^{\infty} p_n e^{i(\alpha+2n)x}\Big) \\
&= -\sum_{n=-\infty}^{\infty} (\alpha+2n)^2 p_n e^{i(\alpha+2n)x} + \sum_{n=-\infty}^{\infty} \Big(\sum_{m=-\infty}^{n} p_m e^{i\alpha x} g_{n-m}\Big) e^{2inx} \\
&= -\sum_{n=-\infty}^{\infty} (\alpha+2n)^2 p_n e^{i(\alpha+2n)x} + \sum_{n=-\infty}^{\infty} \Big(\sum_{m=-\infty}^{n} p_m g_{n-m}\Big) e^{i(\alpha+2n)x} \\
&= \sum_{n=-\infty}^{\infty} \Big[\Big(\sum_{m=-\infty}^{n} p_m g_{n-m}\Big) - (\alpha+2n)^2 p_n\Big] e^{i(\alpha+2n)x} =: \sum_{n=-\infty}^{\infty} C_n e^{i(\alpha+2n)x}
\end{aligned}$$

Since this expression must vanish identically, we have $C_n = 0$ for all n. If we write the coefficient C_n explicitly in terms of p_n and g_n, we have for $-\infty < n < \infty$:

$$\sum_{m=-\infty}^{\infty} [g_{n-m} - (\alpha+2n)^2 \delta_{n,m}] p_m = 0, \tag{4.10}$$

or after multiplication by $[g_0 - (\alpha+2n)^2]^{-1}$, where we have replaced g_0 by λ:

$$\sum_{m=-\infty}^{\infty} \Big[\frac{g_{n-m}}{\lambda - (\alpha+2n)^2} + \delta_{n,m}\Big] p_m = 0, \tag{4.11}$$

where $g_{n-m} = \bar{g}_{m-n}$, $g_0 = 0$. It follows that the determinant:

$$D(\alpha, \lambda) = \left\| \frac{g_{n-m}}{\lambda - (\alpha+2n)^2} + \delta_{n,m} \right\|_{-\infty}^{\infty}$$

converges if $\sum |g_n| < \infty$, except for such values of λ and α for which one of the denominators $\lambda - (\alpha+2n)^2$ vanishes. In such cases, the function may have poles.

4.2.2 Link to the Hill's Discriminant

We also demonstrate how the Hill's discriminant $\Delta(\lambda)$ can be expressed in terms of the Hill's determinant. To obtain this relationship, we use Lemma 4.12.

Lemma 4.12 (Magnus and Winkler [9])**.** *$D(\alpha,\lambda)$, regarded as a function of α, is single valued and analytic for all values of α other than the values:*

$$\alpha = \pm\sqrt{\lambda} - 2n, n = 0, \pm 1, +2, ...,$$

at which the function may have poles. If $\lambda \neq 0$, these poles are (at most) of order one. $D(\alpha,\lambda)$ is periodic in α with period 2, and for $\alpha \to i\infty$, $D(\alpha,\lambda) \to 1$.

Generally speaking, the periodicity of $D(\alpha,\lambda)$ follows from the remark that D remains unchanged if we replace α by $\alpha+2$, while also replacing n by $n-1$ and m by $m-1$:

$$\begin{aligned}
[D(\alpha+2,\lambda)]_{n-1,m-1} &= \left\| \frac{g_{(n-1)-(m-1)}}{\lambda - ((\alpha+2)+2(n-1))^2} + \delta_{n-1,m-1} \right\|_{-\infty}^{\infty} \\
&= \left\| \frac{g_{n-m}}{\lambda - (\alpha+2n)^2} + \delta_{n-1,m-1} \right\|_{-\infty}^{\infty} = [D(\alpha,\lambda)]_{n,m}
\end{aligned}$$

Since both n and m run from $-\infty$ to $+\infty$, the same is also true for $n-1$ and $m-1$. Therefore, we have $D(\alpha+2,\lambda) = D(\alpha,\lambda)$. We also observe that the residues of:

$$\frac{g_{n-m}}{\lambda - (\alpha+2n)^2}$$

at the values $\alpha = \pm\sqrt{\lambda} - 2n$ always add up to zero. This is because if we define:

$$f(\alpha;\lambda) := \frac{g_{n-m}}{\lambda - (\alpha+2n)^2} = \frac{-g_{n-m}}{(\alpha+2n)^2 - \lambda} = \frac{-g_{n-m}}{((\alpha+2n) - \sqrt{\lambda})((\alpha+2n)+\sqrt{\lambda})}$$

$$\alpha_1 := \sqrt{\lambda} - 2n,\ \alpha_2 := -\sqrt{\lambda} - 2n$$

then it follows that:

$$\begin{aligned}
\operatorname{Res}(f(\alpha;\lambda),\alpha) &= \sum_{i=1}^{2} \operatorname{Res}(f(\alpha;\lambda),\alpha_i) \\
&= \lim_{\alpha\to\sqrt{\lambda}-2n} \frac{g_{n-m}(\alpha - (\sqrt{\lambda}-2n))}{\lambda - (\alpha+2n)^2} + \lim_{\alpha\to-\sqrt{\lambda}-2n} \frac{g_{n-m}(\alpha - (-\sqrt{\lambda}-2n))}{\lambda - (\alpha+2n)^2} \\
&= \lim_{\alpha\to\sqrt{\lambda}-2n} \frac{g_{n-m}}{-2(\alpha+2n)} + \lim_{\alpha\to-\sqrt{\lambda}-2n} \frac{g_{n-m}}{-2(\alpha+2n)} \text{ (by L'Hôpital's rule)} \\
&= \frac{g_{n-m}}{-2\sqrt{\lambda}} + \frac{g_{n-m}}{2\sqrt{\lambda}} = 0
\end{aligned}$$

From the periodicity of $D(\alpha,\lambda)$, we have that for $\lambda \neq 0$, all of its residues have the same value K for $\alpha = \sqrt{\lambda} - 2n$ and the value $-K$ for $\alpha = -\sqrt{\lambda} - 2n$. We note the following partial fraction series representation:

$$\pi\cot(\pi z) = \frac{1}{z} + \sum_{n=1}^{\infty} \frac{2z}{z^2 - n^2} \implies \frac{\pi}{2}\cot(\pi z) - \frac{1}{2z} = \sum_{n=1}^{\infty} \frac{z}{z^2-n^2}. \tag{4.13}$$

Using (4.13) and the residue theorem, we can conclude that the function:

$$\begin{aligned} E(\alpha) &:= D(\alpha,\lambda) + \frac{\pi g_{n-m}}{4\sqrt{\lambda}}\cot\Big(\frac{\pi}{2}(\alpha-\sqrt{\lambda})\Big) - \frac{\pi g_{n-m}}{4\sqrt{\lambda}}\cot\Big(\frac{\pi}{2}(\alpha+\sqrt{\lambda})\Big) \\ &= D(\alpha,\lambda) - \frac{\pi K}{2}\Big[\cot\Big(\frac{\pi}{2}(\alpha-\sqrt{\lambda})\Big) - \cot\Big(\frac{\pi}{2}(\alpha+\sqrt{\lambda})\Big)\Big] \end{aligned} \tag{4.14}$$

is an entire function of α with period 2. Since $E(\alpha)$ is bounded in $-1 \leq \mathrm{Re}(\alpha) \leq 1$, then $E(\alpha)$ is a constant, which we shall denote as E. We would like to determine E and K. By letting $\alpha \to i\infty$, we find from Lemma 4.12 that $E = 1$. We cannot determine K explicitly, but we can express it in terms of $D(0,\lambda)$ by letting $\alpha = 0$:

$$\begin{aligned} E(0) &= D(0,\lambda) - \frac{\pi K}{2}\Big[\cot\Big(-\frac{\pi}{2}\sqrt{\lambda}\Big) - \cot\Big(\frac{\pi}{2}\sqrt{\lambda}\Big)\Big] \\ \implies 1 &= D(0,\lambda) - \frac{\pi K}{2}\Big[-\cot\Big(\frac{\pi}{2}\sqrt{\lambda}\Big) - \cot\Big(\frac{\pi}{2}\sqrt{\lambda}\Big)\Big] = D(0,\lambda) + \pi K\cot\Big(\frac{\pi}{2}\sqrt{\lambda}\Big) \\ \implies K &= \frac{1-D(0,\lambda)}{\pi\cot(\frac{\pi}{2}\sqrt{\lambda})} \end{aligned}$$

Hence, this gives the following result:

$$K = \frac{1}{\pi}[1-D(0,\lambda)]\tan\Big(\frac{\pi}{2}\sqrt{\lambda}\Big). \tag{4.15}$$

We apply Theorem 4.6 to (4.11). The infinitely many equations (4.11) are not always equivalent to (4.10), since α may result in a pole. However, we may multiply (4.11) by:

$$\Big(1+\frac{\alpha-\sqrt{\lambda}}{2n}\Big)\Big(1+\frac{\alpha+\sqrt{\lambda}}{2n}\Big) = \frac{(2n+\alpha)^2-\lambda}{4n^2}$$

for $n \neq 0$ and we may multiply (4.11) by $\alpha^2 - \lambda$ for $n = 0$. The determinant of the resulting system must vanish if not all of the p_m's vanish. We note the following Weierstrass product:

$$\frac{\pi}{4}(\alpha^2-\lambda)\prod_{n\neq 0}\Big(1+\frac{\alpha-\sqrt{\lambda}}{2n}\Big)\Big(1+\frac{\alpha+\sqrt{\lambda}}{2n}\Big) = \sin\Big(\frac{\pi}{2}(\alpha-\sqrt{\lambda})\Big)\sin\Big(\frac{\pi}{2}(\alpha+\sqrt{\lambda})\Big). \tag{4.16}$$

Then the existence of a solution of type (4.9) implies that:

$$\sin\Big(\frac{\pi}{2}(\alpha-\sqrt{\lambda})\Big)\sin\Big(\frac{\pi}{2}(\alpha+\sqrt{\lambda})\Big)D(\alpha,\lambda) = 0.$$

Therefore, if we now relate α and λ in a manner such that a solution of type (4.9) exists and (4.16) holds, we find from (4.14) and (4.15) that:

$$4\sin^2\Big(\frac{\pi}{2}\sqrt{\lambda}\Big)D(0,\lambda) = 2 - 2 - \cos(\pi\alpha) = 2 - y_1(\pi;\lambda) - y_2'(\pi;\lambda).$$

Alternatively, we could have computed K in terms of $D(1,\lambda)$. The same argument gives:

$$4\cos^2\Big(\frac{\pi}{2}\sqrt{\lambda}\Big)D(1,\lambda) = 2 + y_1(\pi;\lambda) + y_2'(\pi;\lambda).$$

This leads to the following theorem:

Theorem 4.17 (Magnus [8]). *The Hill's discriminant $\Delta(\lambda)$ can be expressed in two ways as an infinite determinant involving the Fourier coefficients g_n of $V(x)$, which are normalised so that $g_0 = 0$ and $g_{-n} = \bar{g}_n$. In other words, $\Delta(\lambda)$ can be expressed in terms of:*

$$\begin{aligned} D_0(\lambda) &:= D(0,\lambda) = \left\| \frac{g_{n-m}}{\lambda - 4n^2} + \delta_{n,m} \right\|_{-\infty}^{\infty} \\ D_1(\lambda) &:= D(1,\lambda) = \left\| \frac{g_{n-m}}{\lambda - (2n+1)^2} + \delta_{n,m} \right\|_{-\infty}^{\infty} \end{aligned} \quad \textit{such that:} \quad \begin{aligned} 2 - \Delta(\lambda) &= 4\sin^2\left(\frac{\pi}{2}\sqrt{\lambda}\right) D_0(\lambda) \\ 2 + \Delta(\lambda) &= 4\cos^2\left(\frac{\pi}{2}\sqrt{\lambda}\right) D_1(\lambda) \end{aligned}$$

4.2.3 Application of the Fourier Series and Transform

By drawing inspiration from Section 4.2.1, we explore how Fourier series and transforms can be applied to the Hill's equation to obtain a finite difference equation. Ideally, we would like to derive symmetric second order finite difference equations, such that we can obtain infinite Jacobi matrices of the form introduced in Section 3.2.1. We begin by taking the Hill's equation in the standard form:

$$y'' + V(x)y = \lambda y, \tag{4.18}$$

where λ is a parameter and $V(x)$ is a T-periodic function, assumed to be bounded. Suppose that we can write the solution y as a twice-differentiable real Fourier series:

$$y = \sum_{k=0}^{\infty} a_k \cos(kx) + \sum_{k=0}^{\infty} b_k \sin(kx) := y_c + y_s, \tag{4.19}$$

and the potential $V(x)$ can also be expanded in terms of some real Fourier series:

$$V(x) = \sum_{k=0}^{\infty} u_k \cos(kx) + \sum_{k=0}^{\infty} v_k \sin(kx). \tag{4.20}$$

Substituting (4.19) and (4.20) into the Fourier series form of (4.18) gives the resulting equation:

$$\begin{aligned} &-\sum_{k=0}^{\infty} k^2 a_k \cos(kx) - \sum_{k=0}^{\infty} k^2 b_k \sin(kx) \\ &+\Big(\sum_{k=0}^{\infty} u_k \cos(kx) + \sum_{k=0}^{\infty} v_k \sin(kx)\Big)\Big(\sum_{k=0}^{\infty} a_k \cos(kx) + \sum_{k=0}^{\infty} b_k \sin(kx)\Big) \\ &= \lambda \sum_{k=0}^{\infty} a_k \cos(kx) + \lambda \sum_{k=0}^{\infty} b_k \sin(kx) \end{aligned}$$

Suppose that we define the coefficients in terms of their Fourier transform:

$$a_k = \int_0^T y_c \cos(kx)dx,\ b_k = \int_0^T y_s \sin(kx)dx,\ y_k := a_k + b_k.$$

After applying the Fourier transform to both sides of the Fourier series equation, we obtain a second order finite difference equation. We can use this equation to determine a system of orthonormal polynomials.

Example 4.21. Putting the above method into practice, we apply Fourier series and transforms to the Hill's equation with potential $V(x) = 2\cos(x)$, which gives the Mathieu equation:

$$y'' + 2\cos(x)y = \lambda y.$$

Suppose that we can write the solution y as a twice-differentiable real Fourier series:

$$y = \sum_{k=0}^{\infty} a_k \cos(kx) + \sum_{k=0}^{\infty} b_k \sin(kx) := y_c + y_s.$$

The potential is already in real Fourier series form. Using the trigonometric identities:

$$\begin{aligned} \cos(x)\cos(y) &= \frac{1}{2}(\cos(x+y) + \cos(x-y)) \\ \sin(x)\cos(y) &= \frac{1}{2}(\sin(x+y) + \sin(x-y)) \end{aligned} \tag{4.22}$$

it follows that:

$$\begin{aligned} LHS &= -\sum_{k=0}^{\infty} k^2 a_k \cos(kx) - \sum_{k=0}^{\infty} k^2 b_k \sin(kx) + 2\sum_{k=0}^{\infty} a_k \cos(kx)\cos(x) + 2\sum_{k=0}^{\infty} b_k \sin(kx)\cos(x) \\ &= -\sum_{k=0}^{\infty} k^2(a_k \cos(kx) + b_k \sin(kx)) + \sum_{k=0}^{\infty} a_k(\cos((k+1)x) + \cos((k-1)x)) \\ &+ \sum_{k=0}^{\infty} b_k(\sin((k+1)x) + \sin((k-1)x)) \\ RHS &= \lambda \sum_{k=0}^{\infty} a_k \cos(kx) + \lambda \sum_{k=0}^{\infty} b_k \sin(kx) \end{aligned}$$

Suppose that we define:

$$a_k = \int_0^{2\pi} y_c \cos(kx)dx,\ b_k = \int_0^{2\pi} y_s \sin(kx)dx,\ y_k := a_k + b_k.$$

Then taking the Fourier transform of both sides gives:

$$\begin{aligned} (a_{k-1} + b_{k-1}) - k^2(a_k + b_k) + (a_{k+1} + b_{k+1}) &= \lambda(a_k + b_k) \\ \implies y_{k-1} - k^2 y_k + y_{k+1} &= \lambda y_k \end{aligned}$$

Hence, we have obtained a symmetric second order finite difference equation. In Section 4.4.2, we will see that collecting the coefficients of the above recurrence relation will result in the following infinite matrix:

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & \dots \\ 2 & -1 & 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & -4 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & -9 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & -16 & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

As in Example 3.9, we can then obtain a system of orthonormal polynomial solutions, given appropriate initial conditions.

4.2.4 Polynomials of the Bi-Infinite Matrix

In Chapter 3, we uncovered theory that allowed us to generate a system of orthonormal polynomial solutions for symmetric second order finite difference equations as $n \to \infty$. In this section, we would like to explore the notion of polynomials of the bi-infinite Jacobi matrix, in the hope that we can determine whether or not the relevant theory still holds as $n \to -\infty$. We can convert (4.18) to a bi-infinite recurrence relation by taking its complex Fourier transform. We begin by defining a solution in terms of its complex Fourier transform:

$$y_k = \int_0^T y e^{-ikx} dx.$$

By substitution, we have:

$$y'' + V(x)y = \lambda y \implies \int_0^T y'' e^{-ikx} dx + \int_0^T V(x) y e^{-ikx} dx = \lambda \int_0^T y e^{-ikx} dx.$$

Since $V(x)$ is a T-periodic function, then $y(x)$ is also a T-periodic function provided that it is a solution to (4.18). Hence, using integration by parts, the first term reduces to:

$$\begin{aligned}
\int_0^T y'' e^{-ikx} dx &= [y' e^{-ikx}]_0^T + \int_0^T y' ike^{-ikx} dx \\
&= [y' e^{-ikx}]_0^T + ik[y e^{-ikx}]_0^T - \int_0^T k^2 y e^{-ikx} dx \\
&= -k^2 y_k \text{ (given an appropriate choice of } T)
\end{aligned}$$

Suppose that $V(x)$ can be expanded as a complex Fourier series with coefficients v_n:

$$V(x) = \sum_{n=-\infty}^{\infty} v_n e^{inx}.$$

Then the second integral becomes:

$$\begin{aligned}
\int_0^T V(x) y e^{-ikx} dx &= \int_0^T \Big(\sum_{n=-\infty}^{\infty} v_n e^{inx} \Big) y e^{-ikx} dx \\
&= \int_0^T (... + v_{-1} e^{-ix} e^{-ikx} y + v_0 e^{-ikx} y + v_1 e^{ix} e^{-ikx} y + ...) dx \\
&= \int_0^T (... + v_{-1} e^{i(-k-1)x} y + v_0 e^{-ikx} y + v_1 e^{i(-k+1)x} y + ...) dx \\
&= ... + v_{-1} y_{k-1} + v_0 y_k + v_1 y_{k+1} + ...
\end{aligned}$$

Putting this together gives a difference equation of the following form:

$$... + v_{-2} y_{k-2} + v_{-1} y_{k-1} + (v_0 - k^2) y_k + v_1 y_{k+1} + v_2 y_{k+2} + ... = \lambda y_k.$$

By collecting coefficients, we can write this equation as the bi-infinite matrix:

$$\begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & v_0-4 & v_1 & v_2 & v_3 & v_4 & \dots \\ \dots & v_{-1} & v_0-1 & v_1 & v_2 & v_3 & \dots \\ \dots & v_{-2} & v_{-1} & v_0 & v_1 & v_2 & \dots \\ \dots & v_{-3} & v_{-2} & v_{-1} & v_0-1 & v_1 & \dots \\ \dots & v_{-4} & v_{-3} & v_{-2} & v_{-1} & v_0-4 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

Example 4.23. Similarly to Example 3.9, we can generate a system of orthonormal polynomials in the "negative direction". Once again, we will take the example:

$$y_{k-1} - k^2 y_k + y_{k+1} = \lambda y_k.$$

We notice that equating the coefficients of the complex Fourier series does not give us the same issue as the real Fourier series, as explained in Section 4.4.2. Hence we consider the bi-infinite Jacobi matrix:

$$\begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & -4 & 1 & 0 & 0 & 0 & \dots \\ \dots & 1 & -1 & 1 & 0 & 0 & \dots \\ \dots & 0 & 1 & 0 & 1 & 0 & \dots \\ \dots & 0 & 0 & 1 & -1 & 1 & \dots \\ \dots & 0 & 0 & 0 & 1 & -4 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

Using the same initial conditions as before:

$$\begin{aligned} P_0(\lambda) &= 1 & Q_0(\lambda) &= 0 \\ P_1(\lambda) &:= \frac{\lambda - a_0}{b_0} = \lambda & Q_1(\lambda) &:= \frac{1}{b_0} = 1 \end{aligned}$$

we obtain the following system of negative orthonormal polynomials:

$$\begin{aligned} P_0(\lambda) &= 1 & Q_0(\lambda) &= 0 \\ P_{-1}(\lambda) &= 0 & Q_{-1}(\lambda) &= -1 \\ P_{-2}(\lambda) &= -1 & Q_{-2}(\lambda) &= -\lambda - 1 \\ P_{-3}(\lambda) &= -\lambda - 4 & Q_{-3}(\lambda) &= -\lambda^2 - 5\lambda - 3 \\ P_{-4}(\lambda) &= \lambda^2 - 13\lambda - 35 & Q_{-4}(\lambda) &= -\lambda^3 - 14\lambda^2 - 47\lambda - 26 \\ &\dots & &\dots \end{aligned}$$

Already, we notice that Definition 3.6 does not hold, since $P_{-n}(\lambda)$ is no longer a polynomial of exact degree $-n$. Similarly, $Q_{-n}(\lambda)$ is also no longer a polynomial of exact degree $-n-1$. In fact, it seems as though $P_{-n}(\lambda)$ is now a polynomial of exact degree $|-n|-2$ and $Q_{-n}(\lambda)$ is now a polynomial of exact degree $|-n|-1$. We would like to determine whether or not this definition is actually important for our purposes, and whether the theory, such as Jacobi matrices of type C and D, still holds. Our findings will be discussed in Chapter 5.

4.3 Generating Operators Using Jacobi Matrices

4.3.1 Operators Generated by the Moment Problem

As mentioned in Section 3.1, we introduced infinite Jacobi matrices and orthonormal polynomials from a classical moment problem perspective. In this section, we determine how a solution of the moment problem can be used to generate an isometric operator that can be treated as a generalised Fourier series with respect to a basis of orthogonal polynomials.

Definition 4.24 (Isometric Operator)**.** *Suppose that (X, d_X) and (Y, d_Y) are metric spaces. A mapping $U : (X, d_X) \to (Y, d_Y)$ is an isometric operator if:*

$$d_X(x_1, x_2) = d_Y(Ux_1, Ux_2) \text{ for all } x_1, x_2 \in X.$$

Suppose that we know some solution $\sigma(u)$ of the moment problem (3.1). We can construct some L^p_σ ($p \geq 1$) space of σ-measurable functions, such that a significant property of the space is its completeness. In other words, for any Cauchy sequence of functions $f_n(u) \in L^p_\sigma$ where $\lim_{m,n\to\infty} \int_{-\infty}^{\infty} \left| f_n(u) - f_m(u) \right|^p d\sigma(u) = 0$, there exists some function $f(u) \in L^p_\sigma$ such that $\lim_{n\to\infty} \int_{-\infty}^{\infty} \left| f(u) - f_n(u) \right|^p d\sigma(u) = 0$.

We are interested in the case where L^p_σ is a Hilbert space with scalar product:

$$\langle \mathbf{f}, \mathbf{g} \rangle_\sigma = \int_{-\infty}^{\infty} f(u)\overline{g(u)} d\sigma(u),$$

since the orthogonal polynomials $P_k(u)$ will form an orthonormal system in L^2_σ. We can consider the space l^2 (also a Hilbert space) together with L^2_σ. The elements of l^2 will be numerical sequences $\mathbf{x} = \{x_0, x_1, x_2, ...\}$, $\mathbf{y} = \{y_0, y_1, y_2, ...\}$, ... where $\sum_{k=0}^{\infty} |x_k|^2 < \infty$, $\sum_{k=0}^{\infty} |y_k|^2 < \infty$, ... The scalar product in this space can be defined by:

$$\langle \mathbf{x}, \mathbf{y} \rangle = \sum_{k=0}^{\infty} x_k \bar{y}_k.$$

The mapping of l^2 onto L^2_σ is an isometric operator, which we will denote by U.

Definition 4.25 (Finite Vector)**.** *A vector in l^2 is finite if it has only a finite number of components not equal to zero.*

We can define U over all finite vectors $\mathbf{x}$ by the formula:

$$f(u) = U\mathbf{x} = x_0 P_0(u) + x_1 P_1(u) + ... + x_n P_n(u) + ...$$

Since this series terminates in a way such that $f(u)$ is a polynomial with respect to the variable u, then we may write the terminating equality:

$$\int_{-\infty}^{\infty} \left| f(u) \right|^2 d\sigma(u) = \sum_{i,k=0}^{\infty} x_i \bar{x}_k \int_{-\infty}^{\infty} P_i(u) P_k(u) d\sigma(u) = \sum_{k=0}^{\infty} |x_k|^2. \tag{4.26}$$

In other words, we have the equality $\langle \mathbf{f}, \mathbf{f} \rangle_\sigma = \langle \mathbf{x}, \mathbf{x} \rangle$. Similarly, for finite vectors $\mathbf{x}$ and $\mathbf{y}$ such that $f(u) = U\mathbf{x}$ and $g(u) = U\mathbf{y}$, we have $\langle \mathbf{f}, \mathbf{g} \rangle_\sigma = \langle \mathbf{x}, \mathbf{y} \rangle$. For arbitrary, no longer finite vectors of l^2, we can introduce the function:

$$f_n(u) = x_0 P_0(u) + x_1 P_1(u) + ... + x_n P_n(u).$$

Applying (4.26) to the difference $f_n(u) - f_m(u) = x_{m+1}P_{m+1}(u) + ... + x_nP_n(u)$ gives:

$$\int_{-\infty}^{\infty} \left|f_n(u) - f_m(u)\right|^2 d\sigma(u) = \left|x_{m+1}\right|^2 + \left|x_{m+2}\right|^2 + ... + \left|x_n\right|^2 .$$

By Cauchy convergence in L^2_σ, $\lim_{m,n\to\infty} \int_{-\infty}^{\infty} \left|f_n(u) - f_m(u)\right|^2 d\sigma(u) = 0$, and by the completeness of L^2_σ, there exists some unique element $f(u) \in L^2_\sigma$ such that $f(u) = \lim_{\sigma(u)} f_n(u)$. Hence, by the definition of U, we have for any $\mathbf{x} \in l^2$:

$$f(u) = U\mathbf{x} = \lim_{\sigma(u)} \sum_{k=0}^{n} x_k P_k(u).$$

We can confirm that the operator U is isometric, since:

$$\langle \mathbf{x}, \mathbf{y} \rangle = \lim_{n\to\infty} \sum_{k=0}^{n} x_k \bar{y}_k = \lim_{n\to\infty} \langle f_n(u), g_n(u) \rangle_\sigma .$$

This leads to the following theorem:

Theorem 4.27 (Akhiezer [1]). *Any solution $\sigma(u)$ of the moment problem generates an operator U, defined as:*

$$f(u) = U\mathbf{x} = \lim_{\sigma(u)} \sum_{k=0}^{n} x_k P_k(u). \tag{4.28}$$

The domain of this operator is the space l^2. This operator is isometric, satisfying:

$$\langle U\mathbf{x}, U\mathbf{y} \rangle_\sigma = \int_{-\infty}^{\infty} f(u)\overline{g(u)} d\sigma(u) = \sum_{k=0}^{\infty} x_k \bar{y}_k = \langle \mathbf{x}, \mathbf{y} \rangle.$$

The inversion of (4.28) *has the following form, which can be considered as being the generalised Fourier coefficients of $f(u)$:*

$$x_k = \int_{-\infty}^{\infty} f(u) P_k(u) d\sigma(u) \ (k = 0, 1, 2, ...).$$

Example 4.29. We explore the notion of how the Chebyshev moment problem can generate an isometric operator. The classical Chebyshev moment problem has known solutions when we use an $(n-1)$-degree polynomial $R_{k-1}(u)$ to approximate powers of u, also using a supremum norm over the interval $[-1, 1]$. The polynomial $u^k - R_{k-1}(u)$ is a Chebyshev polynomial of the first or second kind with a leading coefficient equal to one, depending on the measure used (Studden [13]). We have the following solutions to the moment problem:

$$\sigma(u) = \begin{cases} \frac{1}{\sqrt{1-u^2}} & \text{when } u^k - R_{k-1}(u) = T_n \text{ (Chebyshev polynomial of the first kind)} \\ \sqrt{1-u^2} & \text{when } u^k - R_{k-1}(u) = U_n \text{ (Chebyshev polynomial of the second kind)} \end{cases}$$

We note that these solutions to the Chebyshev moment problem are also the weights that the Chebyshev polynomials T_n and U_n are orthogonal with respect to:

$$\int_{-1}^{1} T_n(x)T_m(x)\frac{dx}{\sqrt{1-x^2}} = \begin{cases} 0 & n \neq m \\ \pi & n = m = 0 \\ \frac{\pi}{2} & n = m \neq 0 \end{cases}, \quad \int_{-1}^{1} U_n(x)U_m(x)\sqrt{1-x^2}dx = \begin{cases} 0 & n \neq m \\ \frac{\pi}{2} & n = m \end{cases}$$

According to Theorem 4.27, we can use $\sigma(u)$ to generate an isometric operator U (4.28). However, we can go one step further and write an explicit form for U by manipulating generating functions. We note that the Chebyshev polynomials satisfy the following relation:

$$T_n(x) = T_n(\cos(\theta)) = \cos(n\theta),$$

where $x = \cos\theta$. Substituting this into our orthogonality relation gives the following integral:

$$\int_{-1}^{1} \cos(n\theta)\cos(m\theta)\frac{d(\cos(\theta))}{\sqrt{1-\cos^2(\theta)}},$$

hence we can consider $\sigma(u)$ to be the moment problem associated to the operator of multiplication by $\cos(n\theta)$. Let us consider this operator in the following eigenequation:

$$2\cos(x)y = \lambda y. \tag{4.30}$$

We can convert (4.30) to a finite difference equation using the method given in Section 4.2.3. Since the second derivative term y'' is not present, then our associated finite difference equation will be similar to (3.10), except $a_k = 0$. Hence, we have the following finite difference equation:

$$y_{k-1} + y_{k+1} = \lambda y_k. \tag{4.31}$$

We note that (4.31) is extremely close to the Chebyshev recurrence relation (of the first kind), $T_{n-1}(x) + T_{n+1}(x) = 2xT_n(x)$. The infinite Jacobi matrix of (4.31) is given by:

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \dots \\ 2 & 0 & 1 & 0 & 0 & \dots \\ 0 & 1 & 0 & 1 & 0 & \dots \\ 0 & 0 & 1 & 0 & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \tag{4.32}$$

Using (4.31), we can obtain a system of orthonormal polynomials using the initial conditions $y_0 = 1$, $y_1 = x$. We can also derive the generating function $Y(x,t)$ of (4.31) to explicitly solve for $P_k(x)$. Let $Y(x,t) = \sum_{k=0}^{\infty} y_k(x)t^k$. We aim to solve the following expression for Y:

$$\sum_{k=2}^{\infty}(y_k - xy_{k-1} + y_{k-2})t^k = 0.$$

Considering each term, we have:

$$\begin{aligned} \sum_{k=2}^{\infty} y_k t^k &= Y(x,t) - y_0 - y_1 t = Y(x,t) - 1 - xt \\ -x\sum_{k=2}^{\infty} y_{k-1}t^k &= -xt\sum_{k=2}^{\infty} y_{k-1}t^{k-1} = -xt(Y(x,t) - y_0) = -xt(Y(x,t) - 1) \\ \sum_{k=2}^{\infty} y_{k-2}t^k &= t^2\sum_{k=2}^{\infty} y_{k-2}t^{k-2} = t^2 Y(x,t) \end{aligned}$$

Putting all the terms together and solving with respect to Y gives the following:

$$Y(x,t) - 1 - xt - xtY(x,t) + xt + t^2Y(x,t) = 0$$
$$\implies (1 - xt + t^2)Y(x,t) = 1 \implies Y(x,t) = \frac{1}{1 - xt + t^2}$$

We now obtain an expression for y_k, and hence $P_k(x)$, by manipulating the generating function:

$$\begin{aligned}
Y(x,t) = \frac{1}{1-xt+t^2} &= \frac{1}{\sqrt{x^2-4}}\frac{1}{t-\frac{x+\sqrt{x^2-4}}{2}} - \frac{1}{\sqrt{x^2-4}}\frac{1}{t-\frac{x-\sqrt{x^2-4}}{2}} \\
&= \frac{1}{\sqrt{x^2-4}}\Big(-\frac{1}{\frac{x+\sqrt{x^2-4}}{2}-t} + \frac{1}{\frac{x-\sqrt{x^2-4}}{2}-t}\Big) \\
&= \frac{1}{\sqrt{x^2-4}}\Big(\frac{2}{x-\sqrt{x^2-4}}\frac{1}{1-\frac{2t}{x-\sqrt{x^2-4}}} - \frac{2}{x+\sqrt{x^2-4}}\frac{1}{1-\frac{2t}{x+\sqrt{x^2-4}}}\Big) \\
&= \frac{1}{\sqrt{x^2-4}}\Big[\sum_{k=0}^{\infty}\Big(\frac{2}{x-\sqrt{x^2-4}}\Big)^{k+1}t^k - \sum_{k=0}^{\infty}\Big(\frac{2}{x+\sqrt{x^2-4}}\Big)^{k+1}t^k\Big] \ (\because \tfrac{1}{1-t} = \textstyle\sum_{k=0}^{\infty} t^k)
\end{aligned}$$

The expression for y_k is the coefficient of t^k in Y. Therefore, as suggested in Theorem 4.27, we can define the following isometric operator:

$$U\mathbf{x} = \lim_{\sigma(u)} \sum_{k=0}^{n} \frac{x_k}{\sqrt{u^2-4}}\Big[\Big(\frac{2}{u-\sqrt{u^2-4}}\Big)^{k+1} - \Big(\frac{2}{u+\sqrt{u^2-4}}\Big)^{k+1}\Big].$$

We notice that our expression for the isometric operator seems to include multiple instances of the term $\frac{1}{\sqrt{u^2-4}}$, which is close to the solution of the associated Chebyshev moment problem $\sigma(u)$. We can also observe that our solution to the moment problem $\sigma^*(u)$ seems to represent the density of the spectrum of the associated infinite matrix (4.32).

$$\sigma^*(u) = \frac{1}{\sqrt{4-u^2}}. \tag{4.33}$$

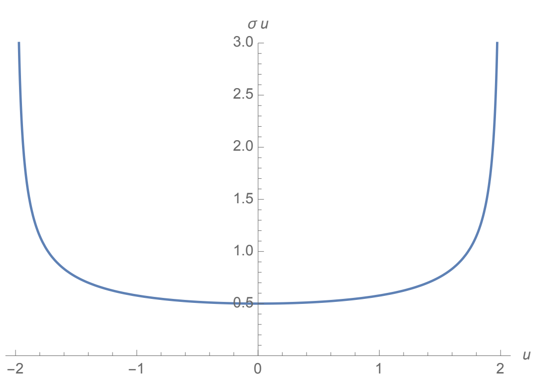

Figure 4.33.1: Plot of the solution (4.33).

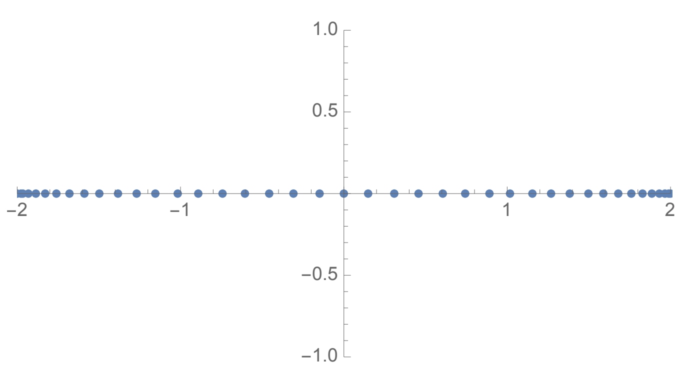

Figure 4.33.2: Spectral density of (4.32).

4.3.2 Symmetry of Jacobi Operators

Definition 4.34 (Jacobi Operator; Teschl [15])**.** *A Jacobi operator is an infinite Jacobi matrix that acts as an operator on a vector.*

In this section, we show that Jacobi operators are symmetric. Hence, we expect the operator generated by an infinite Jacobi matrix to be symmetric as well. We recall the general form of an infinite Jacobi matrix from (3.4), and consider it as the matrix representation of a linear operator A in a separable Hilbert space H.

Definition 4.35 (Separable Hilbert Space)**.** *A Hilbert space is a vector space H with an inner product $\langle \mathbf{f}, \mathbf{g} \rangle$ such that the norm defined by:*

$$|\mathbf{f}| = \sqrt{\langle \mathbf{f}, \mathbf{f} \rangle}$$

turns H into a complete metric space (a metric space where every Cauchy sequence converges). A Hilbert space is separable if and only if it has a countable orthonormal basis.

Suppose that we take an orthonormal basis $\{e_k\}_0^\infty \subseteq H$, and define the linear (Jacobi) operator A for the unit vectors e_k by:

$$Ae_k = b_{k-1}e_{k-1} + a_k e_k + b_k e_{k+1} \ (k = 0, 1, 2, ...; b_{-1} = 0). \tag{4.36}$$

Then A is determined for all finite vectors $\mathbf{g} = \sum_{k=0}^{\infty} x_k e_k$. By (4.36), we have:

$$\begin{aligned} Ae_k = b_{k-1}e_{k-1} + a_k e_k + b_k e_{k+1} &\implies (A - a_k)e_k = b_{k-1}e_{k-1} + b_k e_{k+1} \\ &\implies e_k = (A - a_k)^{-1}(b_{k-1}e_{k-1}) + (A - a_k)^{-1}(b_k e_{k+1}) \end{aligned}$$

By substitution, we have:

$$\begin{aligned} \langle Ae_m, e_n \rangle &= \int (b_{m-1}e_{m-1}e_n + a_m e_m e_n + b_m e_{m+1} e_n) dx \\ \langle e_m, Ae_n \rangle &= \int (b_{n-1}e_{n-1}e_m + a_n e_n e_m + b_n e_{n+1} e_m) dx \\ &= \int (b_{n-1}e_{n-1}[(A - a_m)^{-1}(b_{m-1}e_{m-1}) + (A - a_m)^{-1}(b_m e_{m+1})] + a_n e_m e_n \\ &+ b_n e_{n+1}[(A - a_m)^{-1}(b_{m-1}e_{m-1}) + (A - a_m)^{-1}(b_m e_{m+1})]) dx \\ &= \int ((A - a_m)^{-1}(b_{m-1}e_{m-1})[b_{n-1}e_{n-1} + b_n e_{n+1}] + a_n e_m e_n \\ &+ (A - a_m)^{-1}(b_m e_{m+1})[b_{n-1}e_{n-1} + b_n e_{n+1}]) dx \\ &= \int (b_{m-1}e_{m-1}e_n + a_m e_m e_n + b_m e_{m+1} e_n) dx \end{aligned}$$

This implies that we have the equality $\langle Ae_m, e_n \rangle = \langle e_m, Ae_n \rangle$ $(m, n = 0, 1, 2, ...)$, hence for any two finite vectors $\mathbf{f}$ and $\mathbf{g}$, we have the equality:

$$\langle A\mathbf{f}, \mathbf{g} \rangle = \langle \mathbf{f}, A\mathbf{g} \rangle. \tag{4.37}$$

Since the set of all finite vectors is dense in H, then the Jacobi operator A is symmetric.

4.3.3 The Deficiency Index of an Operator

We can now introduce the deficiency index of an operator, which will be used to classify Jacobi matrices as being of type C or type D (Definition 3.22). We begin by introducing the adjoint operator of A, denoted as A^*. The vector $\mathbf{g} = \sum_{k=0}^{\infty} x_k e_k$ belongs to the domain of A^* if and only if a vector $\mathbf{g}^* = \sum_{k=0}^{\infty} y_k e_k$ exists such that:

$$\langle Ae_k, \mathbf{g} \rangle = \langle e_k, \mathbf{g}^* \rangle \ (k = 0, 1, 2, ...). \tag{4.38}$$

From the identity (4.37), we have that $\langle Ae_k, \mathbf{g} \rangle = \langle e_k, \mathbf{g}^* \rangle$ if and only if $\mathbf{f} = e_k$ and $A\mathbf{g} = \mathbf{g}^*$. Hence, substitution of (4.36) into (4.38) gives:

$$\langle b_{k-1}e_{k-1} + a_k e_k + b_k e_{k+1}, \mathbf{g} \rangle = \langle e_k, \mathbf{g}^* \rangle \implies y_k = b_{k-1}x_{k-1} + a_k x_k + b_k x_{k+1}.$$

Therefore, $\mathbf{g}^*$ is in the domain of A^* if and only if $\sum_{k=0}^{\infty} |b_{k-1}x_{k-1} + a_k x_k + b_k x_{k+1}|^2 < \infty$. We define the deficiency index of A by seeking non-trivial solutions of the equation:

$$A^*\mathbf{g} - \lambda \mathbf{g} = 0, \ \mathrm{Im}(\lambda) \neq 0. \tag{4.39}$$

Let a solution of this equation be the vector $\mathbf{g}$. Then we have:

$$\sum_{k=0}^{\infty} x_k (b_{k-1}e_{k-1} + a_k e_k + b_k e_{k+1}) = \lambda \sum_{k=0}^{\infty} x_k e_k,$$
$$\text{where: } \lambda x_k = b_{k-1}x_{k-1} + a_k x_k + b_k x_{k+1} \ (k = 1, 2, 3, ...), \ \lambda x_0 = a_0 x_0 + b_0 x_1.$$

We have essentially been led to the finite difference equation and boundary condition introduced in Chapter 3. Since this finite difference equation determines the orthogonal polynomials associated with a given Jacobi matrix, it follows that $x_k = cP_k(\lambda)$ $(k = 0, 1, 2, ...)$, where c is a constant. Then (4.39) has a non-trivial solution if and only if $\sum_{k=0}^{\infty} \left|P_k(\lambda)\right|^2 < \infty$, and if this condition is satisfied, then the general solution of (4.39) is the vector:

$$\mathbf{g} = c \sum_{k=0}^{\infty} P_k(\lambda) e_k.$$

Definition 4.40 (Deficiency Index of an Operator; Braeutigam and Mirzoev [3])**.** *Suppose that we have the following positive and negative subspaces of the eigenspace of λ:*

$$\begin{matrix} N_- := \{u \in l^2 : A^* = -\lambda u\} & \multirow{2}{*}{\textit{where:}} & n_- := \dim(N_-) \\ N_+ := \{u \in l^2 : A^* = \lambda u\} & & n_+ := \dim(N_+) \end{matrix}$$

The pair (n_-, n_+) is called the deficiency index of the operator A.

We say that the dimension of the eigenspaces N_- and N_+ is either 0 or 1, depending on the divergence or convergence of the series $\sum_{k=0}^{\infty} \left|P_k(\lambda)\right|^2$. We have the following result:

- If the deficiency index of the operator A is $(0, 0)$, then the Jacobi matrix is of type D.
- If the deficiency index of the operator A is $(1, 1)$, then the Jacobi matrix is of type C.

We have shown that a Jacobi matrix generates a certain symmetric operator. In particular, we found that symmetric operators of deficiency index $(0,0)$ or $(1,1)$ can be generated by matrices of type D or type C respectively. Hence, it seems intuitive to ask questions about the conditions that must exist for the generation of these operators to be possible. In the following sections, we will discuss some of the findings by Marshall Harvey Stone (1932) and Hans Ludwig Hamburger (1944).

4.3.4 Stone's Theorem for Matrices of Type D

Stone proved a theorem about the conditions that must be satisfied by a self-adjoint operator A, such that a Jacobi matrix of type D which generates the operator exists. This theorem involves the notion of a simple spectrum:

Definition 4.41 (Simple Spectrum)**.** *Suppose that A is a linear symmetric operator in n-dimensional space, where $g_1, g_2, ..., g_n$ is the complete system of its eigenvectors and $\lambda_1, \lambda_2, ..., \lambda_n$ are the corresponding eigenvalues. Then $\lambda_1, \lambda_2, ..., \lambda_n$ form the spectrum of the operator. The spectrum is simple if the λ_k are distinct.*

Theorem 4.42 (Stone [12])**.** *Any self-adjoint operator A with simple spectrum is generated by some Jacobi matrix of type D.*

Example 4.43. Throughout the discussion, we have already encountered an example where Stone's Theorem holds: the Mathieu equation. Recall Example 3.9, where we had the finite difference equation:

$$y_{k-1} - k^2 y_k + y_{k+1} = \lambda y_k,$$

and associated infinite matrix, which can be symmetrised to create a Jacobi matrix:

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & ... \\ 2 & -1 & 1 & 0 & 0 & 0 & ... \\ 0 & 1 & -4 & 1 & 0 & 0 & ... \\ 0 & 0 & 1 & -9 & 1 & 0 & ... \\ 0 & 0 & 0 & 1 & -16 & 1 & ... \\ ... & ... & ... & ... & ... & ... & ... \end{pmatrix} \tag{4.44}$$

In Section 4.2.3, we saw that (4.44) was obtained by applying Fourier series and transforms to the Mathieu equation. Hence, we can say that the Mathieu operator generates this infinite Jacobi matrix and vice versa. In Example 3.9, we also obtained the associated orthogonal polynomials of this infinite Jacobi matrix, and in Example 3.24, we determined that (4.44) is a matrix of type D. Hence, by Stone's Theorem, we also expect the Mathieu equation to have a simple spectrum.

We confirmed the simplicity of the periodic spectrum in Example 2.29, where we used the Hill's discriminant and the Oscillation Theorem to highlight intervals of stability, as well as numerically approximate the eigenvalues of the Mathieu operator, which we observed to all have a multiplicity of one. We also remarked that since there seems to be an infinite number of eigenvalues, it was difficult to determine for certain whether or not the spectrum is indeed simple. However, Stone's Theorem now tells us that this is the case. We attempt to verify this by plotting the eigenvalues of a sufficiently large matrix of form (4.44).

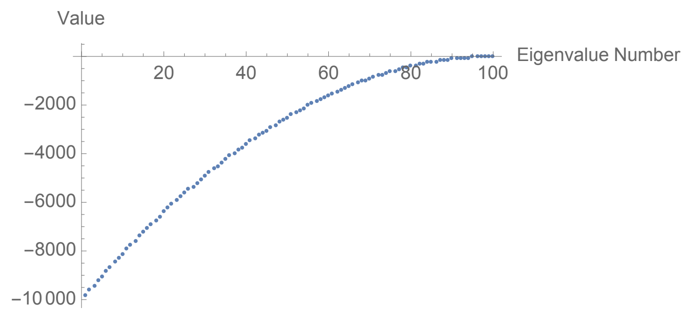

Figure 4.44.1: Spectrum of the 100×100 matrix operator (4.44).

4.3.5 Hamburger's Theorem for Matrices of Type C

Hamburger posed a theorem about the conditions that must be satisfied by a closed symmetric operator A, such that a Jacobi matrix of type C which generates the operator exists. This theorem involves the notion of a simple symmetric operator:

Definition 4.45 (Simple Symmetric Operator; Akhiezer [1])**.** *A symmetric operator A is simple if a space reducing it, in which a part of this operator is a self-adjoint operator, does not exist.*

Definition 4.46 (Space Reducing an Operator; Akhiezer [1])**.** *Let T be any closed linear operator in a Hilbert space H. If the space $H_1 \subset H$ and its orthogonal complement $H \ominus H_1 = H_2$ are invariant subspaces of T, and if a projection into H_1 does not take an element f out of the domain of T, then the space H_1 reduces T.*

Theorem 4.47 (Hamburger [7])**.** *If a closed symmetric operator A is represented by a Jacobi matrix of type C, then A is a simple operator.*

It seems as though examples of matrices of type C, and thus simple symmetric operators generated by such a matrix, are typically difficult to determine. To obtain an example of such a matrix, we use the following theorem:

Theorem 4.48 (Berezansky [2])**.** *Let M be some constant. If:*

$$|a_k| \leq M < \infty \ (k = 1, 2, 3, ...), \tag{4.49}$$

$$\sum_{k=0}^{\infty} \frac{1}{b_k} < \infty \tag{4.50}$$

and if for all k, beginning with a certain value, we have:

$$b_{k-1} b_{k+1} \leq b_k^2, \tag{4.51}$$

then the Jacobi matrix is of type C.

Proof. From Section 4.3.3, we recall that an infinite Jacobi matrix is of type C if the series $\sum_{k=0}^{\infty} \left| P_k(\lambda) \right|^2$ converges. Also recall that we have the finite difference equation:

$$b_{k-1} P_{k-1}(\lambda) + a_k P_k(\lambda) + b_k P_{k+1}(\lambda) = \lambda P_k(\lambda).$$

Then for some fixed $\lambda = \lambda^*$, we have:

$$P_{k+1}(\lambda^*) = \frac{(\lambda^* - a_k)}{b_k} P_k(\lambda^*) - \frac{b_{k-1}}{b_k} P_{k-1}(\lambda^*)$$
$$\implies \sqrt{b_{k+1}}\big|P_{k+1}(\lambda^*)\big| \leq \sqrt{b_{k+1}}\frac{(1+|a_k|)}{b_k}\big|P_k(\lambda^*)\big| + \sqrt{b_{k+1}}\frac{b_{k-1}}{b_k}\big|P_{k-1}(\lambda^*)\big|$$
$$\implies \sqrt{b_{k+1}}\big|P_{k+1}(\lambda^*)\big| \leq \sqrt{b_{k+1}}\frac{(1+|a_k|)\sqrt{b_k}}{b_k\sqrt{b_k}}\big|P_k(\lambda^*)\big| + \sqrt{b_{k+1}}\frac{\sqrt{b_{k-1}}\sqrt{b_{k-1}}}{b_k}\big|P_{k-1}(\lambda^*)\big|$$

By (4.49) and (4.51), we find that, starting from a certain k:

$$\sqrt{b_{k+1}}\big|P_{k+1}(\lambda^*)\big| \leq \frac{1+M}{\sqrt{b_{k-1}b_k}}\sqrt{b_k}\big|P_k(\lambda^*)\big| + \sqrt{b_{k-1}}\big|P_{k-1}(\lambda^*)\big|.$$

Suppose that we define the quantity:

$$N_n = \max_{k=0,1,..,n} \sqrt{b_k}\big|P_k(\lambda^*)\big| \implies N_{n+1} \leq N_n\Big(1 + \frac{1+M}{\sqrt{b_{n-1}b_n}}\Big).$$

Taking into account (4.50), we can conclude that:

$$N_n \leq N_1 \prod_{k=1}^{\infty}\Big(1 + \frac{1+M}{\sqrt{b_{k-1}b_k}}\Big) = N < \infty \ (n = 1, 2, ...)$$
$$\implies \sqrt{b_k}\big|P_k(\lambda^*)\big| \leq N \ (k = 0, 1, 2, ...) \implies \sum_{k=0}^{\infty}\big|P_k(\lambda^*)\big|^2 < \infty. \qquad \square$$

Example 4.52. Let us take the values: $a_k = 0$, $b_k = (k+1)^2$. We note that:

$$\sum_{k=0}^{\infty}\frac{1}{b_k} = \sum_{k=0}^{\infty}\frac{1}{(k+1)^2} = \sum_{k=1}^{\infty}\frac{1}{k^2} = \frac{\pi^2}{6} < \infty$$
$$b_{k-1}b_{k+1} = k^2(k+2)^2 = k^4 + 2k^3 + 4k^2 \leq k^4 + 4k^3 + 6k^2 + 4k + 1 = (k+1)^4 = b_k^2$$

Hence, by Theorem 4.48, we expect these values to result in an infinite Jacobi matrix of type C. This gives the second order finite difference equation $k^2 y_{k-1} + (k+1)^2 y_{k+1} = \lambda y_k$, for which we can write the following infinite Jacobi matrix:

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & ... \\ 1 & 0 & 4 & 0 & 0 & 0 & ... \\ 0 & 4 & 0 & 9 & 0 & 0 & ... \\ 0 & 0 & 9 & 0 & 16 & 0 & ... \\ 0 & 0 & 0 & 16 & 0 & 25 & ... \\ ... & ... & ... & ... & ... & ... & ... \end{pmatrix} \tag{4.53}$$

We can compute orthogonal polynomials of the first and second kind, based on the following initial conditions:

$$P_0(\lambda) = 1 \qquad Q_0(\lambda) = 0$$
$$P_1(\lambda) := \frac{\lambda - a_0}{b_0} = \lambda \quad Q_1(\lambda) := \frac{1}{b_0} = 1$$

By substituting these initial conditions into our finite difference equation, we obtain the following system of orthonormal polynomials and circular contours:

$$
\begin{aligned}
&P_0(\lambda) = 1 && Q_0(\lambda) = 0 \\
&P_1(\lambda) = \lambda && Q_1(\lambda) = 1 \\
&P_2(\lambda) = \frac{1}{4}(\lambda^2 - 1) && Q_2(\lambda) = \frac{\lambda}{4} \\
&P_3(\lambda) = \frac{1}{36}(\lambda^3 - 17\lambda) && Q_3(\lambda) = \frac{1}{36}(\lambda^2 - 16) \\
&P_4(\lambda) = \frac{1}{576}(\lambda^4 - 98\lambda^2 + 81) && Q_4(\lambda) = \frac{1}{576}(\lambda^3 - 97\lambda) \\
&\quad \cdots && \quad \cdots
\end{aligned}
$$

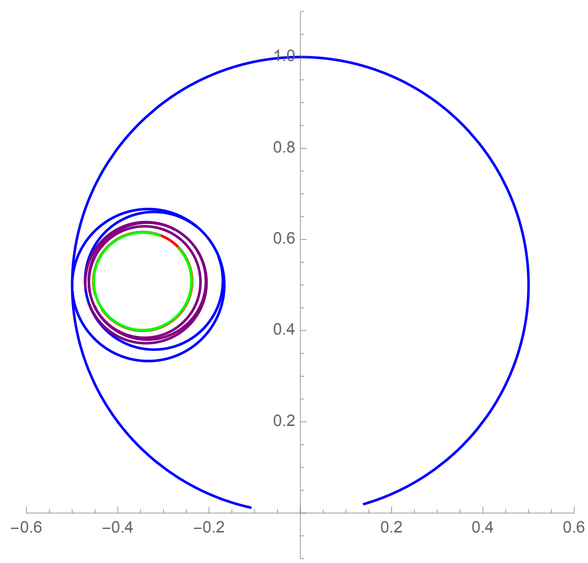

Figure 4.53.1: Circular contours $n = 1, 2, 3, 4, 5, 6, 20, 23, 25$ for the Jacobi matrix (4.53).

In Figure 4.53.1, the blue circles represent $n = 1, 2, 3$, the purple circles represent $n = 4, 5, 6$, the red circle represents $n = 20$, the orange circle represents $n = 23$ and the green circle represents $n = 25$. The red, orange and green circles seem to coincide, or are at least extremely close to one another, implying that we have a limiting circle case. We attempt to verify the convergence of the polynomials numerically:

$$\sum_{k=0}^{20} \left|P_k(i)\right|^2 \approx 0.721 + 0.736i \implies \left|\sum_{k=0}^{20} \left|P_k(i)\right|^2\right| \approx 1.03 < \infty.$$

This suggests that the series evaluated at $\lambda = i$ converges, in accordance with the convergence property proven in Theorem 4.48. Therefore, we believe (4.53) to be a matrix of type C.

We also plot the eigenvalues of (4.53) in an attempt to understand the spectral differences between matrices of type D and C. In particular, since Stone's Theorem states that a matrix of type D should generate a self-adjoint operator with a simple spectrum, we expect this to not be the case for a matrix of type C. In Figure 4.53.2, we observe that there seems to be a certain dimension of the matrix, after which the eigenvalues no longer appear to be distinct.

For example, in the 200×200 Jacobi matrix of form (4.53), a duplicity of eigenvalues seems to occur after the 175th eigenvalue roughly.

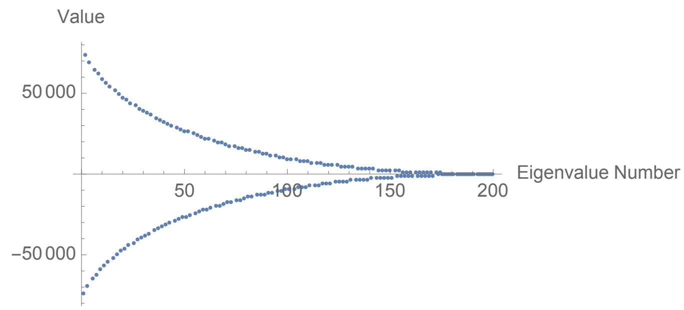

Figure 4.53.2: Spectrum of the 200×200 Jacobi matrix operator (4.53).

4.4 Constructing Series Solutions Using Orthogonal Polynomials

4.4.1 Orthogonal Polynomials as Fourier Coefficients

Let us recall that we have been working with symmetric second order finite difference equations of the form:

$$b_{k-1}y_{k-1} + a_k y_k + b_k y_{k+1} = \lambda y_k. \tag{4.54}$$

In Section 4.2.3, we saw how we can translate the Hill's equation to a finite difference equation of form (4.54), by applying a Fourier transform. Our solutions y_k then form a basis of orthonormal polynomials. In Section 4.3.1, we also saw that the solution to an appropriate moment problem can be used to generate an isometric operator, which can be regarded as the inverse of a generalised Fourier transform with respect to a basis of orthonormal polynomials. Hence, in theory, if a matrix is known to generate some Hill differential operator:

$$Ly := \partial_{xx} y + V(x)y,$$

then we can assume that solutions to the Hill's equation can be written as a Fourier series:

$$y = c_1 \sum_{k=0}^{\infty} y_k \cos(kx) \text{ or } y = c_2 \sum_{k=0}^{\infty} y_k e^{ikx}, \tag{4.55}$$

where c_1, c_2 are constants. In accordance with Theorem 4.27, we should also be able to substitute the orthogonal polynomials $P_k(\lambda^*)$ in place of y_k for some fixed eigenvalue λ^*, since we saw in Example 4.29 that the solution to the moment problem $\sigma(u)$ essentially represents the density of the spectrum.

In this section, we attempt to generate some series solutions to the Hill's equation using orthogonal polynomials. To determine eigenvalues for the evaluation of polynomials, we recall that, as in Example 2.29, we can compute eigenvalues using Hill equation theory. For the time being, we will only consider the polynomials of the first kind, although it is assumed that the method can be applied to the polynomials of the second kind as well. To determine the constants c_1 and c_2, we can impose appropriate initial conditions (2.7). In other words, we let $y(0) = 1$ and $y'(0) = 0$. This gives the following results:

Real Fourier Series:

$$y(0) = 1 \implies c_1 = \frac{1}{\sum_{k=0}^{\infty} P_k(\lambda^*)}$$

Complex Fourier Series:

$$y(0) = 1 \implies c_2 = \frac{1}{\sum_{k=0}^{\infty} P_k(\lambda^*)}$$

We apply this method of obtaining series solutions approximations to periodic solutions of the Hill's equation, in the hope that the discrete and continuous solutions will align well. Since we only apply this method to the Mathieu equation in this essay, we will remark that the success of alignment seems to depend on the symmetry of the potential $V(x)$ chosen.

4.4.2 The Mathieu Equation

In these examples, we will approximate periodic solutions of the Mathieu equation using orthonormal polynomials. First, we recall the Mathieu equation:

$$y'' + 2\cos(x)y = \lambda y.$$

Example 4.56 (Mathieu Equation; Real Fourier Series)**.** As seen in Example 4.21, we can apply Fourier series and transforms to the Mathieu equation to obtain the second order finite difference equation:

$$y_{k-1} - k^2 y_k + y_{k+1} = \lambda y_k.$$

We expect that collecting the coefficients y_k will simply give us an infinite Jacobi matrix of the following form:

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & ... \\ 1 & -1 & 1 & 0 & 0 & 0 & ... \\ 0 & 1 & -4 & 1 & 0 & 0 & ... \\ 0 & 0 & 1 & -9 & 1 & 0 & ... \\ 0 & 0 & 0 & 1 & -16 & 1 & ... \\ ... & ... & ... & ... & ... & ... & ... \end{pmatrix} \tag{4.57}$$

which we can then use to obtain a system of orthonormal polynomials to substitute into our series solution (4.55). However, we should observe that using the real Fourier series representation can pose an issue depending on the starting point of summation. Suppose that our solution is of the form:

$$y = \sum_{k=0}^{\infty} y_k \cos(kx).$$

Then substitution into the Mathieu equation gives:

$$-\sum_{k=0}^{\infty} k^2 y_k \cos(kx) + 2\cos(x) \sum_{k=0}^{\infty} y_k \cos(kx) = \lambda \sum_{k=0}^{\infty} \cos(kx)$$

$$\implies -\sum_{k=0}^{\infty} k^2 y_k \cos(kx) + \sum_{k=0}^{\infty} y_k(\cos((k+1)x) + \cos((k-1)x)) = \lambda \sum_{k=0}^{\infty} \cos(kx) \text{ (by (4.22))}$$

We notice that on the left hand side of this equation, we have:

$$\begin{aligned} LHS &= -(y_1\cos(x) + 4y_2\cos(2x) + ...) + (y_0\cos(x) \\ &\quad + y_1\cos(2x) + ...) + (y_0\cos(-x) + y_1 + y_2\cos(x) + ...) \\ &= y_1 + (2y_0 - y_1)\cos(x) + (y_1 - 4y_2 + y_3)\cos(2x) + ... \end{aligned}$$

which is actually equivalent to an infinite matrix of the form:

$$A := \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & \dots \\ 2 & -1 & 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & -4 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & -9 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & -16 & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \tag{4.58}$$

We note that (4.58) is technically not a Jacobi matrix, since it isn't symmetric. However, as we will see in Section 4.5.2, we can symmetrise (4.58) if required. To summarise the main point of this exercise, we must be careful not to directly substitute the orthogonal polynomials $P_k(\lambda^*)$ obtained from (4.57) into the series solution, since our matrix is really of the form (4.58).

Instead, we recall that the orthogonal polynomials are solutions to the eigenequation (4.54). Therefore, we can define an eigenvector $\mathbf{P}$, where the components of $\mathbf{P}$ are determined by the sequence $P_k(\lambda^*)$. In other words, $\mathbf{P}$ will satisfy the relation $A\mathbf{P} = \mu\mathbf{P}$, for some eigenvalue μ. Let us take the eigenvalue $\lambda^* \approx -16.0318$ as an example. We can evaluate the partial sum:

$$y = \sum_{k=0}^{20} P_k(-16.0318)\cos(kx). \tag{4.59}$$

We can plot (4.59) as a function of x (Figure 4.59.1). We also plot the periodic solution to the Mathieu equation evaluated at $\lambda = -16.0318$ for comparison (Figure 4.59.2). As we can see in the figures, the shape of the discrete approximation seems to match the periodic solution of the Mathieu equation. However, as explained in Section 4.4.1, we need to multiply our discrete solution by an extra sum to align the discrete and continuous solutions (Figure 4.59.3):

$$\frac{1}{\sum_{k=0}^{20} P_k(-16.0318)} \approx -1.03178.$$

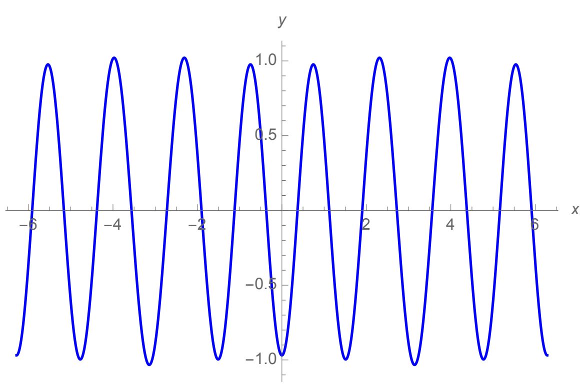

Figure 4.59.1: Plot of (4.59).

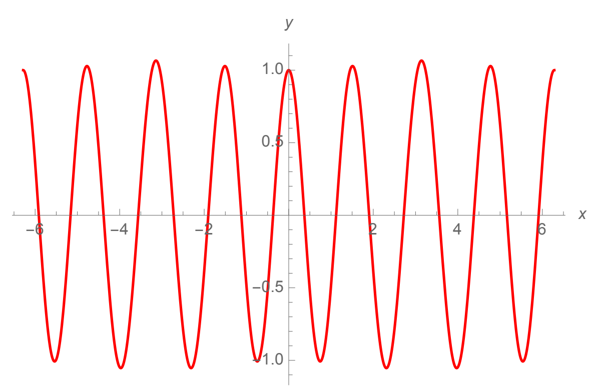

Figure 4.59.2: Periodic solution of $y'' + 2\cos(x)y = -16.0318y$, obtained numerically.

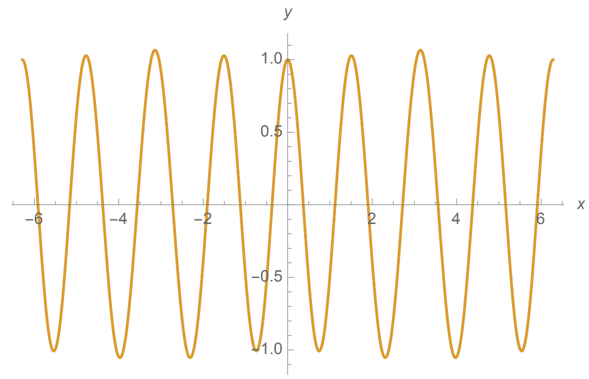

Figure 4.59.3: Comparison of the real Fourier series solution and the periodic solution of the Mathieu equation obtained numerically.

Example 4.60 (Mathieu Equation; Complex Fourier Series)**.** Applying the method given in Section 4.2.4 allows us to obtain a bi-infinite Jacobi matrix of the form:

$$B := \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & -4 & 1 & 0 & 0 & 0 & \dots \\ \dots & 1 & -1 & 1 & 0 & 0 & \dots \\ \dots & 0 & 1 & 0 & 1 & 0 & \dots \\ \dots & 0 & 0 & 1 & -1 & 1 & \dots \\ \dots & 0 & 0 & 0 & 1 & -4 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

As explained in Example 4.56, we take $P_k(\lambda^*)$ to be the components of an eigenvector of B. Let us take the eigenvalue $\lambda^* \approx -1.70727$ as an example. We can evaluate the partial sum:

$$y = \sum_{k=-40}^{40} P_k(-1.70727)e^{ikx}. \tag{4.61}$$

We can plot (4.61) as a function of x (Figure 4.61.1). We also plot the periodic solution to the Mathieu equation evaluated at $\lambda = -1.70727$ for comparison (Figure 4.61.2). As explained in Section 4.4.1, we also need to multiply our discrete solution by an extra sum in order to align the discrete and continuous solutions (Figure 4.61.3):

$$\frac{1}{\sum_{k=-40}^{40} P_k(-1.70727)} \approx -0.970578.$$

4.5 Differential Equations with Known Orthogonal Polynomials

4.5.1 Orthogonal Polynomials as Eigenvectors of the Fourier Transform

There are several examples of differential equations that have associated recurrence relations that return a system of orthogonal polynomials, such as the Hermite and Legendre differential

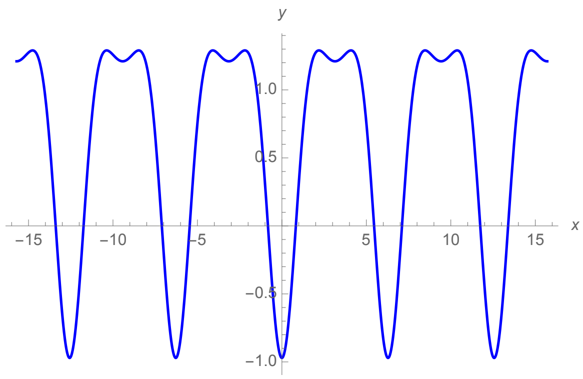

Figure 4.61.1: Plot of (4.61).

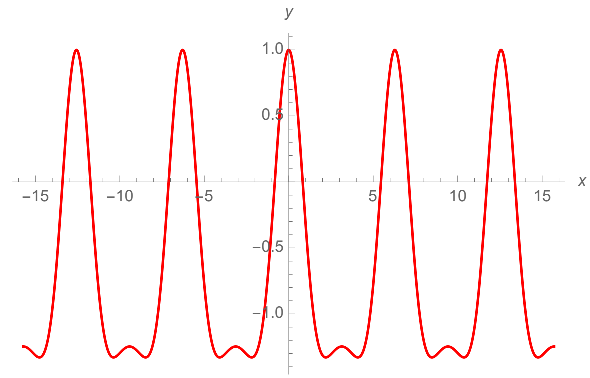

Figure 4.61.2: Periodic solution of $y'' + 2\cos(x)y = -1.70727y$, obtained numerically.

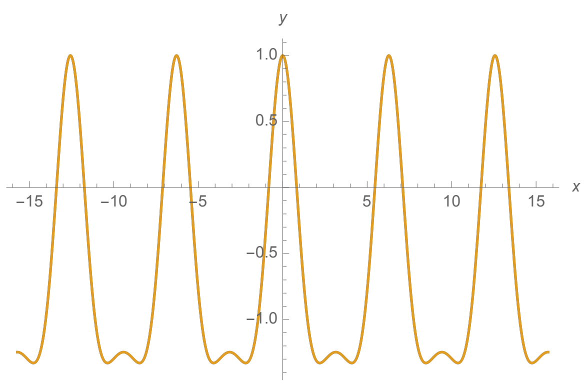

Figure 4.61.3: Comparison of the complex Fourier series solution and the periodic solution of the Mathieu equation obtained numerically.

equations. However, it may not be clear as to how these different components were derived, as well as how they may be related. The examples in this section will hopefully serve as an attempt to make some of these connections clearer. We reiterate the point raised in Example 4.56, that symmetric second order finite difference equations of the form:

$$b_{k-1}y_{k-1} + a_k y_k + b_k y_{k+1} = \lambda y_k \tag{4.62}$$

can be viewed as eigenequations $Ay_k = \lambda y_k$, if we define the operator A by:

$$Ay_k := b_{k-1}y_{k-1} + a_k y_k + b_k y_{k+1}.$$

This suggests that our solutions of (4.62), which are the orthogonal polynomials y_k, will form a basis for the eigenvectors of A. We also recall that in Section 4.2.3, we obtained these finite difference equations by applying the Fourier transform to a periodic ordinary differential equation. Hence, in a way we can consider A to merely be the Fourier transform operator.

In this section, we apply the theory introduced in Chapters 3 and 4 to make sense of how orthogonal polynomials can be considered as eigenfunctions of the continuous Fourier transform, as well as how Stone's Theorem, for example, can be applied to non-symmetric matrices to determine information about the spectrum of the associated operator.

Ideally, we would like to link these results to the theory introduced in Chapter 2. In particular, it would be interesting to see if we can determine an appropriate periodic ordinary differential equation such that we can apply the method of Section 4.4.1 to obtain a fairly accurate series solution to the periodic ordinary differential equation. However, the method of obtaining such an equation is currently uncertain, as merely taking the inverse Fourier transform of the associated symmetric second order finite difference equations typically results in ordinary differential equations with non-periodic solutions.

4.5.2 Hermite Differential Equation

The Hermite differential equation is $y'' - 2xy' + 2ny = 0$. If $n = 0, 1, 2, 3, ...$, then the solution of the Hermite differential equation is given by the Hermite polynomial $H_n(x)$ (Szegö [14]). These polynomials satisfy the following recurrence relations:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{4.63}$$
$$H_n'(x) = 2nH_{n-1}(x) \tag{4.64}$$

It is also known that the Hermite polynomials are orthogonal with respect to the weight e^{-x^2}:

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x)H_n(x)dx = \begin{cases} 0 & \text{if } m \neq n \\ 2^n n!\sqrt{\pi} & \text{if } m = n \end{cases}$$

Example 4.65 (Hermite Differential Equation; Infinite Jacobi Matrix)**.** Let us consider (4.63), treating x as an eigenvalue. Writing the left hand side as an infinite matrix gives:

$$\begin{pmatrix} 0 & 1 & 0 & ... & ... & ... \\ 2 & 0 & 1 & 0 & ... & ... \\ 0 & 4 & 0 & 1 & 0 & ... \\ ... & 0 & 6 & 0 & 1 & ... \\ ... & ... & 0 & 8 & 0 & ... \\ ... & ... & ... & ... & ... & ... \end{pmatrix} \tag{4.66}$$

In order to apply the theory introduced in Chapters 3 and 4, we need to convert (4.66) to an infinite Jacobi matrix. To symmetrise (4.66), we consider the quadratic form acting on it.

Definition 4.67 (Quadratic Form)**.** *A quadratic form is a function $f : \mathbb{R}^n \to \mathbb{R}$ such that $f(\mathbf{x}) = \mathbf{x}^T Q\mathbf{x}$, where $\mathbf{x} = (x_1, x_2, ..., x_n)$ and Q is an $n \times n$ matrix.*

It follows that we can actually replace a non-symmetric matrix Q with $\frac{1}{2}(Q + Q^T)$ such that:

$$\mathbf{x}^T Q\mathbf{x} = \frac{1}{2}\mathbf{x}^T(Q + Q^T)\mathbf{x}.$$

Hence, performing this transformation on (4.66) gives:

$$\begin{pmatrix} 0 & \frac{3}{2} & 0 & ... & ... & ... \\ \frac{3}{2} & 0 & \frac{5}{2} & 0 & ... & ... \\ 0 & \frac{5}{2} & 0 & \frac{7}{2} & 0 & ... \\ ... & 0 & \frac{7}{2} & 0 & \frac{9}{2} & ... \\ ... & ... & 0 & \frac{9}{2} & 0 & ... \\ ... & ... & ... & ... & ... & ... \end{pmatrix} \tag{4.68}$$

Example 4.69 (Hermite Differential Equation; (Positive) Orthonormal Polynomials)**.** The Jacobi matrix (4.68) allows us to define a symmetric second order finite difference equation:

$$\frac{2k+1}{2}y_{k-1} + \frac{2k+3}{2}y_{k+1} = 2xy_k. \tag{4.70}$$

As explained in Chapter 3, if we set the following initial conditions:

$$\begin{aligned} &P_0(x) = 1 && Q_0(x) = 0 \\ &P_1(x) := \frac{2x - a_0}{b_0} = \frac{2x}{\frac{3}{2}} = \frac{4x}{3} && Q_1(x) := \frac{1}{b_0} = \frac{1}{\frac{3}{2}} = \frac{2}{3} \end{aligned}$$

then we can generate a system of orthonormal polynomials of the first and second kind:

$$\begin{aligned} &P_0(x) = 1 && Q_0(x) = 0 \\ &P_1(x) = \frac{4x}{3} && Q_1(x) = \frac{2}{3} \\ &P_2(x) = \frac{1}{15}(16x^2 - 9) && Q_2(x) = \frac{8x}{15} \\ &P_3(x) = \frac{8}{105}(8x^3 - 17x) && Q_3(x) = \frac{2}{105}(16x^2 - 25) \\ &P_4(x) = \frac{1}{945}(256x^4 - 1328x^2 + 441) && Q_4(x) = \frac{16}{945}(8x^3 - 37x) \\ &P_5(x) = \frac{4}{10395}(256x^5 - 2624x^3 + 3195x) && Q_5(x) = \frac{2}{10395}(256x^4 - 2480x^2 + 2025) \\ &\quad\dots && \quad\dots \end{aligned}$$

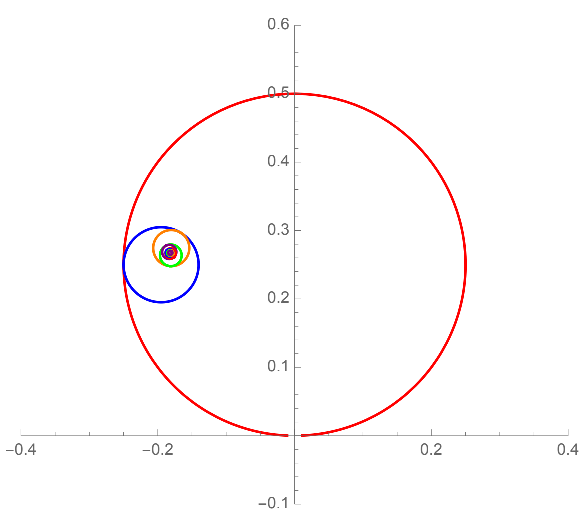

Figure 4.70.1: Contours (4.70), $n = 1, ..., 10$.

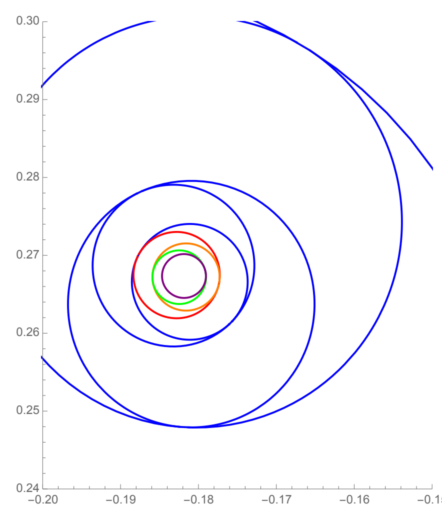

Figure 4.70.2: Contours for (4.70), magnified. Coloured circles represent $n = 7, ..., 10$.

We plot the circular contours obtained by these polynomials for $n = 1, ..., 10$ (Figure 4.70.1). Since the circles continue to decrease in radius as $n \to \infty$, we suspect that the circular contours converge to a point and (4.68) is a Jacobi matrix of type D. Similarly to Example 3.24, we verify the classification of (4.68) by checking that:

$$\sum_{k=0}^{\infty} \left|P_k(\lambda)\right|^2 \text{ diverges.}$$

In the interest of computational efficiency, we have the following result for the partial sum:

$$\sum_{k=0}^{20} \left|P_k(i)\right|^2 \approx -5.272 \times 10^7 + 1.061 \times 10^7 i \implies \left|\sum_{k=0}^{20} \left|P_k(i)\right|^2\right| \approx 5.377 \times 10^7.$$

Therefore, the series evaluated at $\lambda = i$ diverges. Hence, by Stone's Theorem, this suggests that (4.68) will generate some self-adjoint operator with a simple spectrum. We can start to see that the spectrum is simple if we compute the eigenvalues of Jacobi matrices of type (4.68) as they increase in size. For example, we have the following computations:

Size of $n \times n$ matrix	Eigenvalues
2	$\pm\frac{3}{2} = \pm 1.5$
3	$\pm\sqrt{\frac{17}{2}} \approx \pm 2.915, 0$
4	$\pm\sqrt{\frac{83}{8} + \frac{5\sqrt{205}}{8}} \approx \pm 4.396, \pm\frac{1}{2}\sqrt{\frac{1}{2}(83 - 5\sqrt{205})} \approx 1.194$
5	$-\frac{1}{2}\sqrt{82 \pm \sqrt{3529}} \approx -5.897, -2.496, \frac{\sqrt{82\pm\sqrt{3529}}}{2} \approx 5.946, 2.377, 0$

We aim to verify the simplicity of the spectrum by plotting the eigenvalues of a large enough matrix of type (4.68) (Figure 4.70.3). However, due to computational inefficiency, it was difficult to compute the spectrum of a matrix of size larger than 50×50. Nonetheless, we still expect Stone's Theorem to hold.

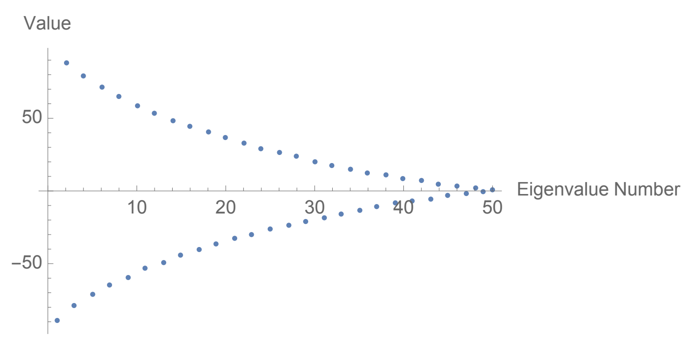

Figure 4.70.3: Spectrum of the 50×50 modified Hermite Jacobi matrix operator (4.68).

Example 4.71 (Hermite Differential Equation; (Negative) Orthonormal Polynomials)**.** We also compute the polynomials of the bi-infinite Jacobi matrix. We expect to see that Stone's theorem still holds in the negative sub-eigenspace (Definition 4.40). Using the same initial conditions as before, we can generate the following system of orthonormal polynomials:

$$\begin{aligned}
P_0(x) &= 1 & Q_0(x) &= 0\\
P_{-1}(x) &= 0 & Q_{-1}(x) &= -2\\
P_{-2}(x) &= 1 & Q_{-2}(x) &= 8x\\
P_{-3}(x) &= -\frac{4x}{3} & Q_{-3}(x) &= \frac{1}{3}(32x^2 - 2)\\
P_{-4}(x) &= \frac{1}{15}(16x^2 - 9) & Q_{-4}(x) &= \frac{16}{15}(8x^3 - 5x)\\
P_{-5}(x) &= -\frac{8}{105}(8x^3 - 17x) & Q_{-5}(x) &= -\frac{2}{105}(256x^4 - 560x^2 + 25)\\
&\cdots & &\cdots
\end{aligned}$$

As in Example 4.23, we notice that $P_{-n}(x)$ seems to be a polynomial of exact degree $|-n|-2$ and $Q_{-n}(x)$ seems to be a polynomial of exact degree $|-n|-1$. By comparison with $P_n(x)$, we also notice that $P_{-n}(x) = -P_{|-n|-2}(x)$. This suggests that there is some symmetry in the Fourier coefficients, if we take the polynomials of the first kind to be the generalised Fourier coefficients of the solution. However, there does not seem to be a discernible relationship between $Q_{-n}(x)$ and $Q_n(x)$.

We also plot the circular contours obtained by these polynomials for $n = -1, ..., -9$ (Figure 4.71.1). However, we should disregard the contour for $n = -1$, since this is defined as:

$$\omega_{-1}(x;\tau) = -\frac{Q_{-1}(x) - \tau Q_{-2}(x)}{P_{-1}(x) - \tau P_{-2}(x)} = -\frac{-2 - \tau 8x}{0 - \tau}.$$

This gives a linear function with respect to τ, hence the solution extends across all the real numbers and we no longer have a circular contour. Disregarding $n = -1$, we once again observe that the circular contours seem to converge to a point as $n \to -\infty$. We numerically verify this by determining that:

$$\sum_{k=-20}^{0} \left|P_k(i)\right|^2 \approx -1.88 \times 10^{26} - 6.860 \times 10^{22} i \implies \left|\sum_{k=-20}^{0} \left|P_k(i)\right|^2\right| \approx 1.88 \times 10^{24}.$$

Therefore, the series evaluated at $\lambda = i$ diverges and we believe that the bi-infinite Jacobi matrix is of type D in the negative direction. This suggests that Stone's Theorem will hold in the negative sub-eigenspace as well, which is perhaps not surprising due to the definition of the deficiency index of the operator being a pair (n_-, n_+), where $n_- = n_+$.

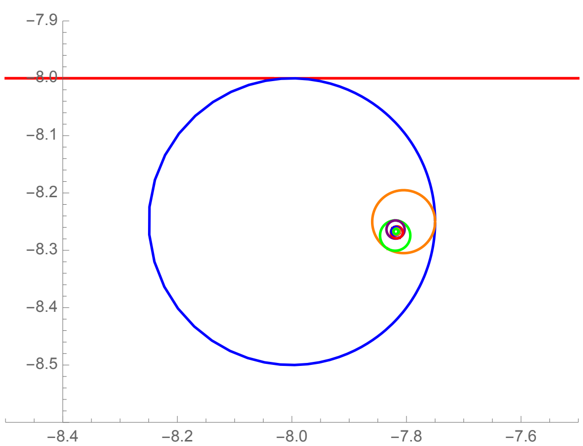

Figure 4.71.1: Contours (4.70), $n = -1, ..., -9$.

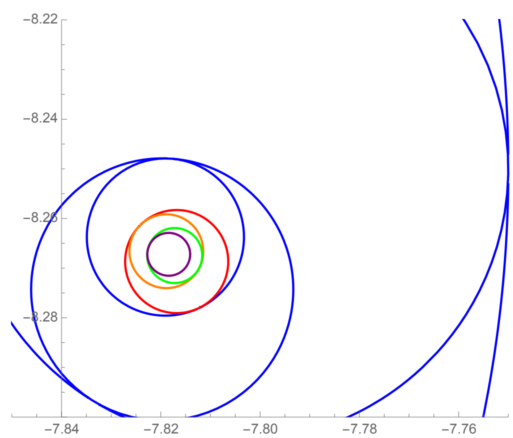

Figure 4.71.2: Contours for (4.70), magnified. Coloured circles represent $n = -6, ..., -9$.

4.5.3 Legendre Differential Equation

The Legendre differential equation is $(1 - x^2)y'' - 2xy' + n(n+1)y = 0$. The Legendre polynomials are orthogonal polynomials that are eigenfunctions of the Hermitian differential operator (Szegö [14]):

$$\frac{d}{dx}\left[(1 - x^2)\frac{d}{dx}P(x)\right] = -\lambda P(x),$$

where the eigenvalue $\lambda = n(n+1)$ for $n = 0, 1, 2, 3, ...$ It is also known that the Legendre polynomials are orthogonal with respect to the L^2 norm on the interval $-1 \leq x \leq 1$:

$$\int_{-1}^{1} P_m(x)P_n(x)dx = \frac{2}{2n+1}\delta_{mn}.$$

Example 4.72 (Legendre Differential Equation; Infinite Jacobi Matrix)**.** The Legendre polynomials satisfy the following recurrence relation:

$$nP_{n-1}(x) - 2nxP_n(x) + (n+1)P_{n+1}(x) = xP_n(x), \tag{4.73}$$

where we will treat x as an eigenvalue. Writing the left hand side as an infinite matrix gives:

$$\begin{pmatrix} 0 & 1 & 0 & ... & ... & ... \\ 1 & -2x & 2 & 0 & ... & ... \\ 0 & 2 & -4x & 3 & 0 & ... \\ ... & 0 & 3 & -6x & 4 & ... \\ ... & ... & 0 & 4 & -8x & ... \\ ... & ... & ... & ... & ... & ... \end{pmatrix} \tag{4.74}$$

We observe that (4.74) is already a symmetric matrix, hence (4.73) is a symmetric second order finite difference equation to which we can apply the theory of Chapters 3 and 4.

Example 4.75 (Legendre Differential Equation; (Positive) Orthonormal Polynomials)**.** As explained in Chapter 3, if we set the following initial conditions:

$$\begin{aligned} P_0(x) &= 1 & Q_0(x) &= 0 \\ P_1(x) &:= \frac{x - a_0}{b_0} = \frac{x}{1} = x & Q_1(x) &:= \frac{1}{b_0} = \frac{1}{1} = 1 \end{aligned}$$

then we can generate a system of orthonormal polynomials of the first and second kind:

$$\begin{aligned} P_0(x) &= 1 & Q_0(x) &= 0 \\ P_1(x) &= x & Q_1(x) &= 1 \\ P_2(x) &= \frac{1}{2}(3x^2 - 1) & Q_2(x) &= \frac{3x}{2} \\ P_3(x) &= \frac{1}{2}(5x^3 - 3x) & Q_3(x) &= \frac{5x^2}{2} - \frac{2}{3} \\ P_4(x) &= \frac{1}{8}(35x^4 - 30x^2 + 3) & Q_4(x) &= \frac{5}{24}(21x^3 - 11x) \\ P_5(x) &= \frac{1}{8}(63x^5 - 70x^3 + 15x) & Q_5(x) &= \frac{63x^4}{8} - \frac{49x^2}{8} + \frac{8}{15} \\ &... & &... \end{aligned}$$

In this case, the polynomials $P_n(x)$ are the same as the already-established Legendre polynomials, since the Legendre recurrence relation was symmetric to begin with. We plot the circular contours obtained by these polynomials for $n = 1, ..., 7$ (Figure 4.75.1). Since the circles continue to decrease in radius as $n \to \infty$, we observe that the circular contours converge to a point and believe (4.74) to be a Jacobi matrix of type D. Similarly to Example 3.24, we

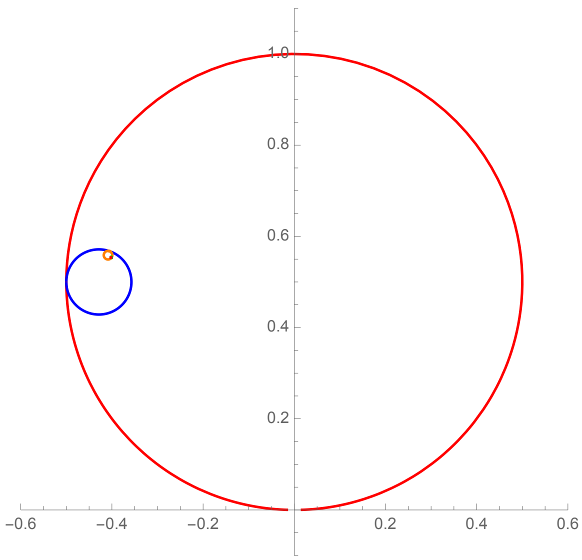

Figure 4.75.1: Circular contours for (4.73).

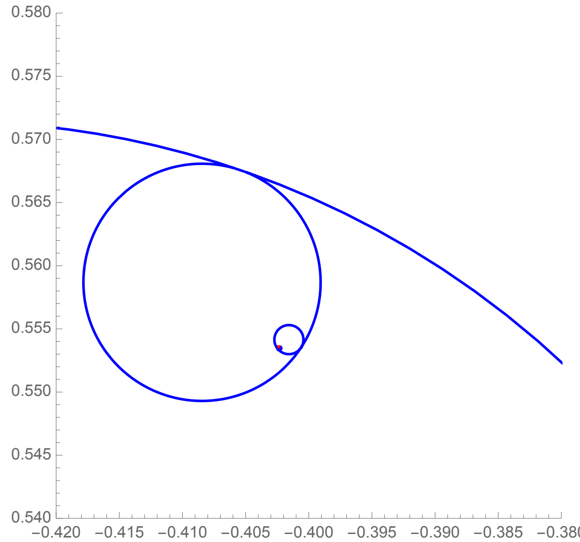

Figure 4.75.2: Circular contours for (4.73), magnified. Coloured point represents $n = 7$.

verify the classification of (4.74) by checking that:

$$\sum_{k=0}^{\infty} \left|P_k(\lambda)\right|^2 \text{ diverges.}$$

In the interest of computational efficiency, we have the following result for the partial sum:

$$\sum_{k=0}^{20} \left|P_k(i)\right|^2 = -189626.$$

Therefore, the series evaluated at $\lambda = i$ diverges. Hence, by Stone's Theorem, this suggests that (4.74) will generate some self-adjoint operator with a simple spectrum. We can start to see that the spectrum is simple if we attempt to compute the eigenvalues of our Jacobi matrices of type (4.74) as they increase in size. For example, we have the following computations:

Size of $n \times n$ matrix	Eigenvalues
2	$\pm\frac{1}{\sqrt{3}} \approx \pm 0.577$
3	$\pm\sqrt{\frac{3}{5}} \approx \pm 0.775, 0$
4	$\pm\sqrt{\frac{1}{35}(15 - 2\sqrt{30})} \approx \pm 0.340, \pm\sqrt{\frac{1}{35}(15 + 2\sqrt{30})} \approx \pm 0.861$
5	$\pm\frac{1}{3}\sqrt{\frac{1}{7}(35 - 2\sqrt{70})} \approx \pm 0.538, \pm\frac{1}{3}\sqrt{\frac{1}{7}(35 + 2\sqrt{70})} \approx 0.906, 0$

We aim to verify the simplicity of the spectrum by plotting the eigenvalues of a large matrix of type (4.74) (Figure 4.75.3). It seems as though Stone's Theorem holds, with the eigenvalues being extremely close in value to one another as the dimension of the matrix increases.

Example 4.76 (Legendre Differential Equation; Associated Isometric Operator)**.** Fortunately, the solution of the Legendre recurrence relation can be used to determine a generating function with a nice closed form. In Example 4.29, we saw how the generating function can be used to

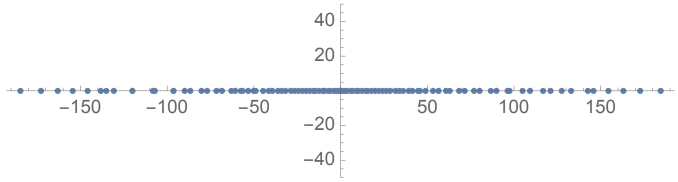

Figure 4.75.3: Spectrum of the 100×100 Legendre Jacobi matrix operator (4.74).

determine an explicit form for the isometric operator generated by the infinite Jacobi matrix (4.74). To begin with, we determine the Legendre generating function:

$$Y(x,t) = \sum_{k=0}^{\infty} y_k t^k,$$

where t is a parameter. In this case, we recall that our finite sequence y_k satisfies (4.73):

$$(k+1)y_{k+1} - (2k+1)xy_k + ky_{k-1} = 0 \implies ky_k - (2k-1)xy_{k-1} + (k-1)y_{k-2} = 0.$$

We also recall the initial conditions for our polynomials $P_n(x)$, which were $y_0 = 1$ and $y_1 = x$. By considering derivatives with respect to t, we have:

$$\frac{dY(x,t)}{dt} = \sum_{k=1}^{\infty} ky_k t^{k-1} \implies t\frac{dY(x,t)}{dt} = \sum_{k=1}^{\infty} ky_k t^k.$$

We aim to solve the following expression for Y:

$$\sum_{k=2}^{\infty} (ky_k - (2k-1)xy_{k-1} + (k-1)y_{k-2})t^k = 0.$$

Considering each term, we have:

$$\begin{aligned}
\sum_{k=2}^{\infty} ky_k t^k &= t\frac{dY(x,t)}{dt} - y_1 t = t\frac{dY(x,t)}{dt} - xt \\
-2x\sum_{k=2}^{\infty} ky_{k-1} t^k &= -2x\sum_{k=1}^{\infty} (k+1)y_k t^{k+1} = -2xt^2\frac{dY(x,t)}{dt} - 2xtY(x,t) + 2xt \\
x\sum_{k=2}^{\infty} y_{k-1} t^k &= xt\sum_{k=2}^{\infty} y_{k-1} t^{k-1} = xt(Y(x,t) - y_0) = xt(Y(x,t) - 1) \\
\sum_{k=2}^{\infty} ky_{k-2} t^k &= \sum_{k=0}^{\infty} (k+2)y_k t^{k+2} = t^2\sum_{k=0}^{\infty} ky_k t^k + 2t^2\sum_{k=0}^{\infty} y_k t^k = t^3\frac{dY(x,t)}{dt} + 2t^2 Y(x,t) \\
-\sum_{k=2}^{\infty} y_{k-2} t^k &= -t^2\sum_{k=2}^{\infty} y_{k-2} t^{k-2} = -t^2 Y(x,t)
\end{aligned}$$

Putting all the terms together gives us the following relation:

$$t\frac{dY(x,t)}{dt} - xt - 2xt^2\frac{dY(x,t)}{dt} - 2xtY(x,t) + 2xt + xtY(x,t) - xt + t^3\frac{dY(x,t)}{dt} + 2t^2 Y(x,t) - t^2 Y(x,t) = 0.$$

Simplifying and solving with respect to Y gives:

$$\begin{aligned}
(t^3 - 2xt^2 + t)\frac{dY(x,t)}{dt} + (t^2 - xt)Y(x,t) = 0 \implies \frac{Y'}{Y} &= \frac{-t+x}{t^2 - 2xt + 1} \\
\implies \int \frac{Y'}{Y} dt &= -\frac{1}{2}\int \frac{-2(-t+x)}{t^2 - 2xt + 1} dt \\
\implies \log(Y) &= -\frac{1}{2}\log(t^2 - 2xt + 1) + C \\
\implies Y(x,t) &= \frac{C}{\sqrt{t^2 - 2xt + 1}}
\end{aligned}$$

where C is an arbitrary constant. To determine the value of the constant, we impose the initial condition $Y(x,0) = y_0 = 1$. Hence, we consider the case where $C = 1$. We note that this corresponds with the canonical form of the generating function for the Legendre polynomials (of the first kind):

$$\sum_{n=0}^{\infty} P_n(x)u^n = \frac{1}{\sqrt{1 - 2xu + u^2}}. \tag{4.77}$$

As in Theorem 4.27, we now aim to determine an isometric operator of the form (4.28). We obtain an explicit form for the operator by considering the coefficient of u^n in the series (4.77):

$$\begin{aligned}
Y(x,t) &= \frac{1}{\sqrt{t^2 - 2xt + 1}} = \frac{1}{\sqrt{t - (x + \sqrt{x^2 - 1})}\sqrt{t - (x - \sqrt{x^2 - 1})}} \\
&= \frac{1}{\sqrt{2\sqrt{x^2 - 1}}}\frac{1}{\sqrt{t - (x + \sqrt{x^2 - 1})}} - \frac{i}{\sqrt{2\sqrt{x^2 - 1}}}\frac{1}{\sqrt{t - (x - \sqrt{x^2 - 1})}} \\
&= \frac{1}{\sqrt{2\sqrt{x^2 - 1}}}\Big(\sqrt{\frac{-1}{(x + \sqrt{x^2 - 1}) - t}} + \sqrt{\frac{1}{(x - \sqrt{x^2 - 1}) - t}}\Big) \\
&= \frac{1}{\sqrt{2\sqrt{x^2 - 1}}}\Big(\sqrt{\frac{-1}{x + \sqrt{x^2 - 1}}}\frac{1}{\sqrt{1 - \frac{t}{x + \sqrt{x^2 - 1}}}} + \sqrt{\frac{1}{x - \sqrt{x^2 - 1}}}\frac{1}{1 - \frac{t}{\sqrt{x - \sqrt{x^2 - 1}}}}\Big) \\
&= \frac{1}{\sqrt{2\sqrt{x^2 - 1}}}\Big[\sum_{k=0}^{\infty} i\binom{k - \frac{1}{2}}{k}\Big(\frac{1}{\sqrt{x + \sqrt{x^2 - 1}}}\Big)^{k+1} t^k + \sum_{k=0}^{\infty}\binom{k - \frac{1}{2}}{k}\Big(\frac{1}{\sqrt{x - \sqrt{x^2 - 1}}}\Big)^{k+1} t^k\Big]
\end{aligned}$$

We note that the last line of the derivation comes from the identity:

$$\frac{1}{(1-t)^c} = \sum_{k=0}^{\infty}\binom{c + k - 1}{k} t^k.$$

Therefore, we can define the following isometric operator:

$$U\mathbf{x} = \lim_{\sigma(u)}\sum_{k=0}^{n}\binom{k - \frac{1}{2}}{k}\frac{x_k}{\sqrt{2\sqrt{x^2 - 1}}}\Big[i\Big(\frac{1}{\sqrt{x + \sqrt{x^2 - 1}}}\Big)^{k+1} + \Big(\frac{1}{\sqrt{x - \sqrt{x^2 - 1}}}\Big)^{k+1}\Big].$$

Since the term $\sqrt{x^2 - 1}$ occurs frequently, we can hypothesise that the solution to the supposed "Legendre moment problem of the first kind" would be:

$$\sigma^*(u) = \frac{1}{\sqrt{x^2 - 1}}. \tag{4.78}$$

Interestingly, if we plot this function (Figure 4.78.1), and compare the nature of the function against the spectrum of the Legendre Jacobi matrix (Figure 4.75.3), we notice that, once again, $\sigma^*(u)$ seems to represent the density of the spectrum.

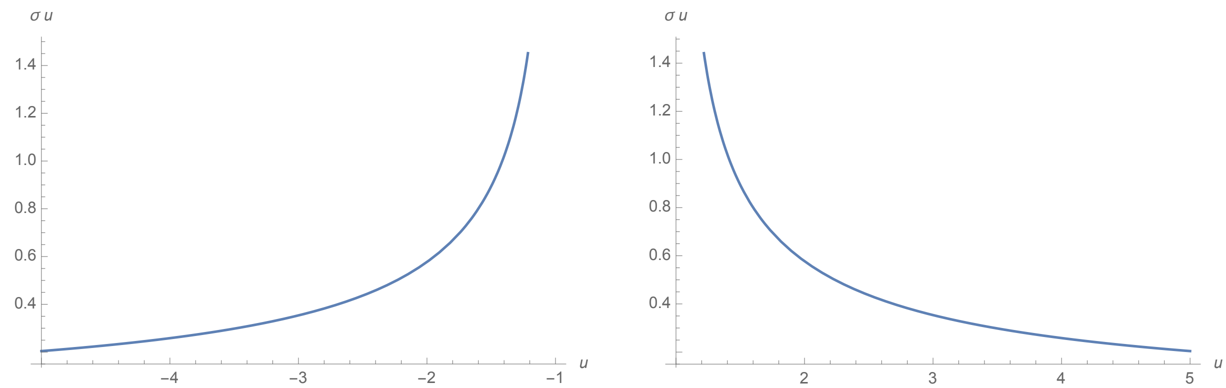

Figure 4.78.1: Plot of (4.78), after restricting the domain.

4.6 Return to the Moment Problem

In this section, we aim to bring together some of the concepts previously discussed; such as the moment problem, infinite Jacobi matrices, orthogonal polynomials, Fourier series and Fourier transforms, to discuss the overall picture. Although there are likely many more intricacies concerning this topic, we currently understand these components to be connected by the relationship described in Figure 4.79.1.

From our study of Akhiezer's "The Classical Moment Problem" [1], it is believed that if we know some solution of the moment problem, then we can use the associated positive sequence to construct a system of orthonormal polynomials that are solutions to a symmetric second order finite difference equation. This difference equation can be represented in an infinite Jacobi matrix form, which is essentially a matrix representation of the Fourier transform. We can then construct an isometric operator that is a generalised Fourier series with an orthonormal basis in L^2_σ. The inversion of this operator gives a sequence in l^2.

Let us recall the Chebyshev moment problem of the first kind. In Example 4.29, we saw that the solution is given by the measure over the interval $[-1, 1]$, $\sigma(u) = \frac{1}{\sqrt{1-u^2}}$, which we can use to compute generalised moments of order k:

$$s_k = \int_{-1}^{1} u^k \frac{du}{\sqrt{1-u^2}}.$$

Doing so numerically gives the positive sequence: $\pi, 0, \frac{\pi}{2}, 0, \frac{3\pi}{8}, 0, \frac{5\pi}{16}, 0, \frac{35\pi}{128}, \ldots$ The positive sequence elements without the factor of π also form the sequence $\binom{2n}{n}/4^n$ (Sloane [10]). If we substitute this sequence into a Hankel matrix, and use Hankel determinants to define a system of orthogonal polynomials, we obtain results such as:

$$P_0(x) = 1, P_1(x) = \sqrt{2}x, P_2(x) = \frac{8}{\pi^3}(2x^2 - 1), P_3(x) = \frac{64}{\pi^4}(8x^3 - 6x), \ldots$$

Applying the definitions for the coefficients a_k and b_k (Section 3.2.3) gives the equation:

$$\frac{1}{2}y_{k-1} + \frac{1}{2}y_{k+1} = xy_k \implies y_{k-1} + y_{k+1} = 2xy_k, \tag{4.79}$$

which, as we saw in Example 4.29, is the same as the so-called Chebyshev recurrence relation. Taking the complex Fourier transform of (4.79) tells us that this finite difference equation corresponds to the eigenequation $\cos(x)y = \lambda y$. By Theorem 4.27, there exists some isometric operator U in the form (4.28) that maps elements in l^2 to L^2_σ. As in Example 4.29, we can obtain an explicit form for this operator by manipulating the generating function for y_k:

$$Y(x,t) = \frac{1}{1 - 4xt + t^2}.$$

By following the same method as in Example 4.29, we obtain the explicit form of the operator:

$$U\mathbf{x} = \lim_{\sigma(u)} \sum_{k=0}^{n} \frac{x_k}{2\sqrt{u^2-1}} \left[\left(\frac{1}{2u - \sqrt{u^2-1}} \right)^{k+1} - \left(\frac{1}{2u + \sqrt{u^2-1}} \right)^{k+1} \right].$$

As expected, this isometric operator essentially allows us to recover the solution to the Chebyshev moment problem. We also recall that $\sigma(u)$ provides us with information about the spectral density of the associated matrix operator, which we can possibly connect to the spectrum of the associated differential operator or eigenequation.

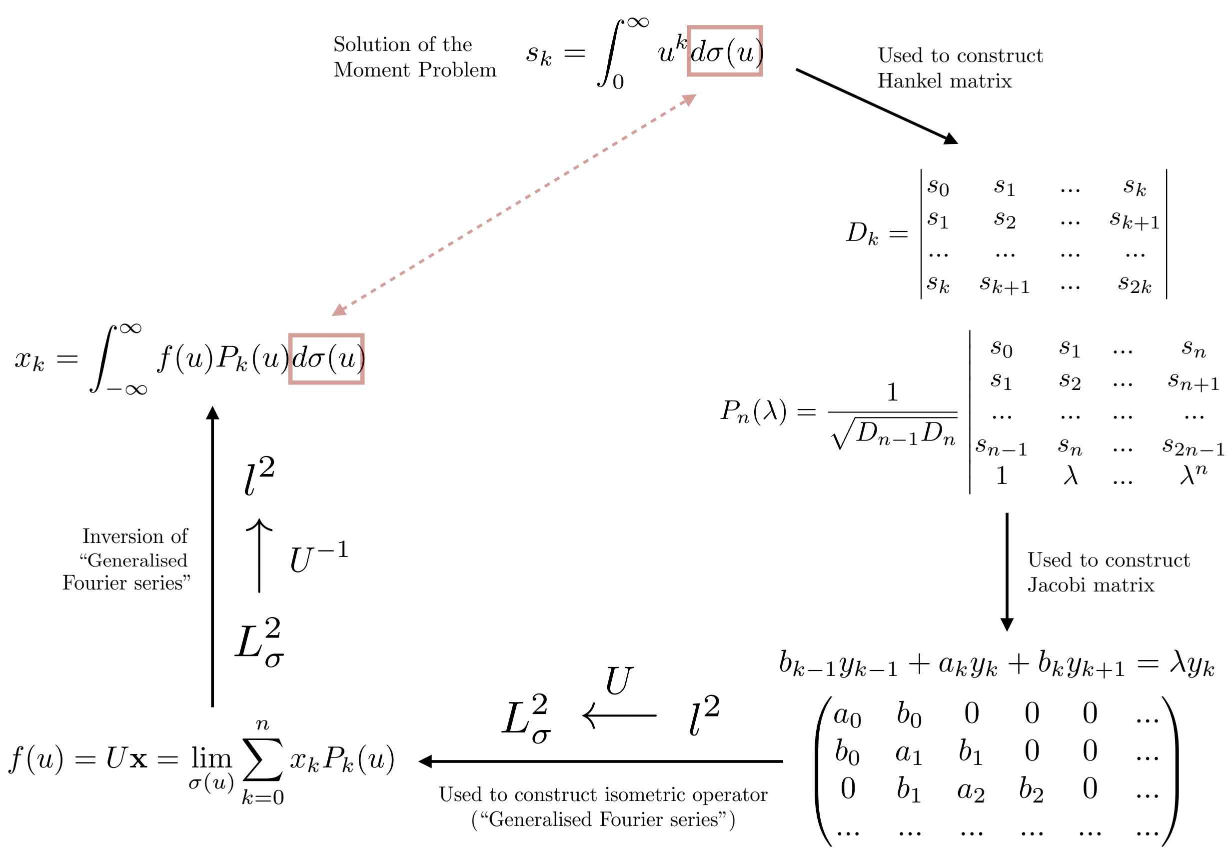

Figure 4.79.1: Connections between concepts introduced throughout the discussion.

Chapter 5

Conclusion

The fields of second order symmetric linear ordinary differential equations and second order symmetric linear finite difference equations are indeed closely related. This connection is made more explicit if we consider second order symmetric finite difference equations to be the discrete analogue of second order periodic ordinary differential equations, while the system of orthonormal polynomial solutions can be used to generate series solutions to the periodic ordinary differential equation.

In Chapter 4, we found that we can translate a second order periodic ordinary differential equation to a second order symmetric finite difference equation by writing solutions in terms of their Fourier series and applying a Fourier transform. This allowed us to define an infinite Jacobi matrix and system of orthonormal polynomials. We also extended the polynomials to a bi-infinite matrix and found that the discrete theory, particularly Stone's Theorem, still seems to hold, although more investigations would need to be conducted before any definitive claims can be made. Since there is typically a linear discontinuity at $n = -1$ due to the initial condition $Q_0(x) = 0$, it seems as though Stone's Theorem holds in the positive or negative subspace only, as defined in Definition 4.40.

One particular question that we were interested in was the spectral information of the differential operator that we could obtain from the infinite Jacobi matrix. This information came in the form of Stone's Theorem for matrices of type D (limiting point case) and Hamburger's Theorem for matrices of type C (limiting circle case). In particular, we found that Stone's Theorem gives the remarkable result that any self-adjoint operator with simple spectrum is generated by some Jacobi matrix of type D. This is an example of a powerful tool that could allow us to determine information about the infinite periodic spectrum of a differential operator, as briefly alluded to in Example 2.29.

Furthermore, we determined how an isometric operator can be generated by the classical moment problem, which came as a result of constructing our infinite Jacobi matrices in Chapter 3. We also saw that since the Jacobi operator is symmetric, then the operator generated by the matrix is expected to be symmetric as well. By the construction of this operator, we can consider the orthogonal polynomials evaluated at some fixed eigenvalue to be generalised Fourier coefficients of some series solution to the associated periodic ordinary differential equation. In addition, we saw that the sequence of orthonormal polynomials can act as the basis for an eigenvector of the Fourier transform operator.

There are many directions in which this research can be continued. To begin with, it seems as though the existing literature on orthogonal polynomials is lacking in information concerning infinite Jacobi matrices and their classification. Not many examples of Jacobi matrices and their associated operators seem to be widely accessible, and most examples of Jacobi matrices obtained by personal investigation were of the limiting point case. It would be interesting to understand more about the limiting circle case, and in particular, if there are any other theorems such as Theorem 4.48 that allow us to construct Jacobi matrices of type C.

If we compare the circular contours for the modified Hermite recurrence relation (Figure 4.70.1) and the Legendre recurrence relation (Figure 4.75.1), for example, we can see that the Legendre polynomials seem to converge to a point faster than the modified Hermite polynomials. It may also be an area of interest to determine whether or not the rate at which the contours converge plays a role in uncovering spectral information about the associated operator.

In Section 4.4, we determined that the system of orthonormal polynomials can be used to construct series solutions to the periodic ordinary differential equation. However, while the results were promising for the Mathieu equation, the series solution is not always an optimal approximation for the periodic solution. Hence, future research could be conducted around the improvement of such series solutions.

In addition, the theory of infinite Jacobi matrices can be linked to the theory of continued fractions. Instead of a positive sequence, we can introduce the formal power series:

$$\frac{s_0}{z} + \frac{s_1}{z^2} + ... + \frac{s_m}{z^{m+1}} + ... \ (s_0 = 1),$$

and instead of an infinite Jacobi matrix, we can introduce the formal infinite continued fraction:

$$\frac{1}{z - a_0 - \frac{b_0^2}{z - a_1 - \frac{b_1^2}{z - a_2 - ...}}}.$$

Then given appropriate notation, these components can be used to define convergents (approximating fractions), such that the numerators and denominators of these convergents satisfy finite difference equations of the form $Y_{k+1} = (z - a_k)Y_k - b_{k-1}^2 Y_{k-1}$. Another avenue of research could be an investigation into the role that continued fractions play in the world of orthogonal polynomials, and thus possibly periodic ordinary differential equations as well.

Overall, it seems as though this problem of finding connections between the discrete and continuous fields contains many complexities, many of which we still have yet to fully understand. In this essay, we considered the second order symmetric case only, but perhaps there are also connected results between differential equations and finite difference equations of higher order, or those that are not necessarily symmetric. The potential applications of this research are widespread, as understanding the connections between these problems could allow for more efficient computation or the numerical approximation of solutions to ordinary differential equations that are typically difficult to solve.

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Appendices (Code)

Appendix A. Hill's Discriminant and Eigenvalues

```
clear all;

% We wish to solve the ODE: y''+(lambda+2cos(x))y=0.
% Rewriting as a first order system gives: y'=u, u'=-(lambda+V(x))y.
% Initial conditions: y_1(0)=1, y_1'(0)=0, y_2(0)=0, y_2'(0)=1.

period=2*pi; % Period of the potential
lstart=-5; % Start of eigenvalue interval
lend=50; % End of eigenvalue interval
lambda=lstart:0.05:lend;
% Plot lines at Delta = pm 2 for comparison
n2=zeros(1,length(lambda));
p2=zeros(1,length(lambda));
for i=1:length(lambda)
    n2(1,i)=-2;
    p2(1,i)=2;
end
delta=zeros(1,length(lambda));
% In this case, we use MATLAB ode45 to solve the ODE
for l=lambda
    [t,y]=ode45(@(t,y)solve_1(t,y,l), [0 period], [1 0 0 1]);
    index=find(lambda==l);
    delta(1,index)=y(length(t),1)+y(length(t),4); % Trace of monodromy
end

% Plot the Hill's discriminant
plot(lambda,delta,lambda,n2,'red',lambda,p2,'red')
title(['Plot of \Delta(' num2str(period) ',\lambda)']);
xlabel('\lambda');
ylabel('\Delta(2\pi,\lambda)');
axis([lstart lend -3 3])

% Save and store the eigenvalues
index=1;
for i=1:length(delta)
    % Save eigenvalues that round up to pm 2
    if round(delta(1,i))==-2 || round(delta(1,i))==2
        eigenval(1,index)=lambda(1,i);
        index=index+1;
    end
end
```

Appendix B. Orthogonal Polynomials and Circular Contours

```
Clear["`*"]
```

```
(*Generate an infinite Jacobi matrix for the Hermite polynomials*)
```

```
mm[n_] := DiagonalMatrix[Table[(2 * i + 1) / 2, {i, 1, n - 1}], -1] +
  DiagonalMatrix[Table[0, {k, 1, n}]] +
  DiagonalMatrix[Table[(2 * i + 1) / 2, {i, 1, n - 1}], 1]
```

```
mm[5] // MatrixForm
```

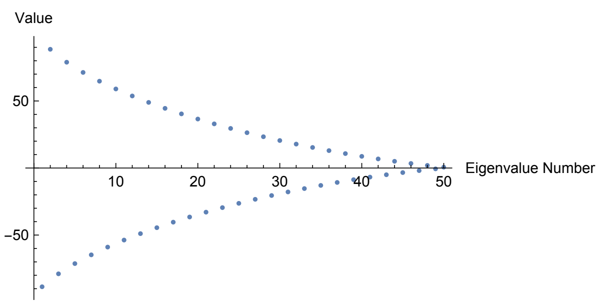
$$\begin{pmatrix} 0 & \frac{3}{2} & 0 & 0 & 0 \\ \frac{3}{2} & 0 & \frac{5}{2} & 0 & 0 \\ 0 & \frac{5}{2} & 0 & \frac{7}{2} & 0 \\ 0 & 0 & \frac{7}{2} & 0 & \frac{9}{2} \\ 0 & 0 & 0 & \frac{9}{2} & 0 \end{pmatrix}$$

```
(*Compute eigenvalues and plot spectrum of the Jacobi matrix*)
```

```
Eigenvalues[mm[5]]
```

$$\left\{-\frac{1}{2}\sqrt{82+\sqrt{3529}},\ \frac{\sqrt{82+\sqrt{3529}}}{2},\ -\frac{1}{2}\sqrt{82-\sqrt{3529}},\ \frac{\sqrt{82-\sqrt{3529}}}{2},\ 0\right\}$$

```
ListPlot[Eigenvalues[mm[50]], AxesLabel → {"Eigenvalue Number", "Value"}]
```




```
(*Compute positive polynomials of the first kind*)
```

```
h1[k_] = RSolve[{((2 k + 3) / 2) * p[k + 1] - 2 * x * p[k] + ((2 k + 1) / 2) * p[k - 1] == 0,
    p[0] == 1, p[1] == (4 * x) / 3}, p[k], k];
For[m = 0, m < 6, m++, Print[Simplify[h1[m]]]]
```

$\{\{p[0] \to 1\}\}$

$$\left\{\left\{p[1] \to \frac{4x}{3}\right\}\right\}$$

$$\left\{\left\{p[2] \to \frac{1}{15}\left(-9+16x^2\right)\right\}\right\}$$

$$\left\{\left\{p[3] \to \frac{8}{105}x\left(-17+8x^2\right)\right\}\right\}$$

$$\left\{\left\{p[4] \to \frac{1}{945}\left(441-1328x^2+256x^4\right)\right\}\right\}$$

$$\left\{\left\{p[5] \to \frac{4x\left(3195-2624x^2+256x^4\right)}{10\,395}\right\}\right\}$$

```
(*Compute positive polynomials of the second kind*)
```

```
h2[k_] = RSolve[{((2 k + 3) / 2) * q[k + 1] - 2 * x * q[k] + ((2 k + 1) / 2) * q[k - 1] == 0,
     q[0] == 0, q[1] == 2 / 3}, q[k], k];
For[m = 0, m < 6, m++, Print[Simplify[h2[m]]]]
```

$\{\{q[0] \to 0\}\}$

$\left\{\left\{q[1] \to \frac{2}{3}\right\}\right\}$

$\left\{\left\{q[2] \to \frac{8\,x}{15}\right\}\right\}$

$\left\{\left\{q[3] \to \frac{2}{105}\,(-25 + 16\,x^2)\right\}\right\}$

$\left\{\left\{q[4] \to \frac{16}{945}\,x\,(-37 + 8\,x^2)\right\}\right\}$

$\left\{\left\{q[5] \to \frac{2\,(2025 - 2480\,x^2 + 256\,x^4)}{10\,395}\right\}\right\}$

```
(*Circular contours for the positive polynomials*)
```

$$\text{w1}[x\_,\ \tau\_] := -\left(\left(\frac{2}{3}\right) \Big/ \left(\frac{4\,x}{3} - \tau * (1)\right)\right);$$

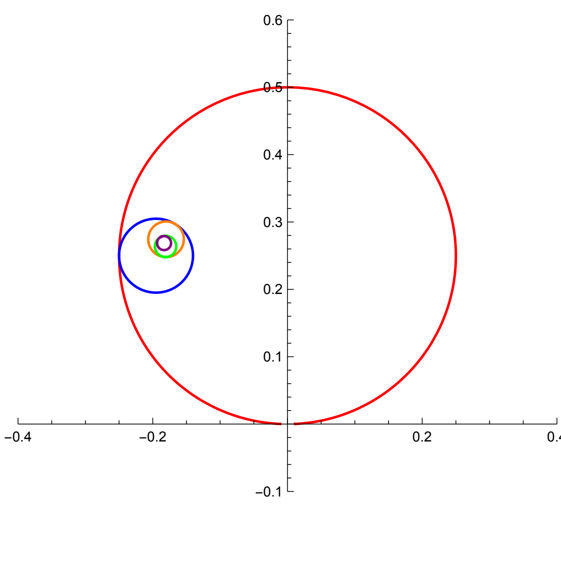
$$\text{w2}[x\_,\ \tau\_] := -\left(\left(\frac{8\,x}{15} - \tau * \left(\frac{2}{3}\right)\right) \Big/ \left(\frac{1}{15}\left(-9 + 16\,x^2\right) - \tau * \left(\frac{4\,x}{3}\right)\right)\right);$$

$$\text{w3}[x\_,\ \tau\_] := -\left(\left(\frac{2}{105}\left(-25 + 16\,x^2\right) - \tau * \left(\frac{8\,x}{15}\right)\right) \Big/ \left(\frac{8}{105}\,x\left(-17 + 8\,x^2\right) - \tau * \left(\frac{1}{15}\left(-9 + 16\,x^2\right)\right)\right)\right);$$

$$\text{w4}[x\_,\ \tau\_] := -\left(\left(\frac{16}{945}\,x\left(-37 + 8\,x^2\right) - \tau * \left(\frac{2}{105}\left(-25 + 16\,x^2\right)\right)\right) \Big/ \left(\frac{1}{945}\left(441 - 1328\,x^2 + 256\,x^4\right) - \tau * \left(\frac{8}{105}\,x\left(-17 + 8\,x^2\right)\right)\right)\right);$$

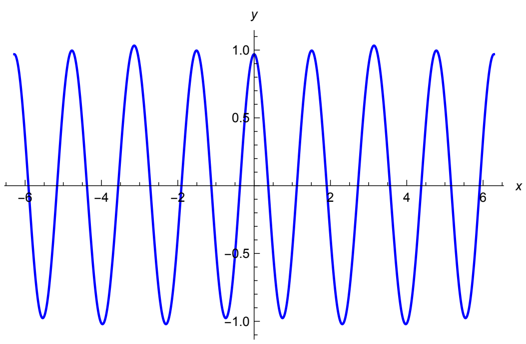
$$\text{w5}[x\_,\ \tau\_] := -\left(\left(\frac{2\left(2025 - 2480\,x^2 + 256\,x^4\right)}{10\,395} - \tau * \left(\frac{16}{945}\,x\left(-37 + 8\,x^2\right)\right)\right) \Big/ \left(\frac{4\,x\left(3195 - 2624\,x^2 + 256\,x^4\right)}{10\,395} - \tau * \left(\frac{1}{945}\left(441 - 1328\,x^2 + 256\,x^4\right)\right)\right)\right);$$

```
(*Plot circular contours*)
Show[ParametricPlot[{Re[w1[1 + I, τ]], Im[w1[1 + I, τ]]},
   {τ, -60, 60}, PlotRange → {{-0.4, 0.4}, {-0.1, 0.6}}, PlotStyle → Red],
 ParametricPlot[{Re[w2[1 + I, τ]], Im[w2[1 + I, τ]]}, {τ, -60, 60},
  PlotRange → {{-0.4, 0.4}, {-0.1, 0.6}}, PlotStyle → Blue],
 ParametricPlot[{Re[w3[1 + I, τ]], Im[w3[1 + I, τ]]}, {τ, -60, 60},
  PlotRange → {{-0.4, 0.4}, {-0.1, 0.6}}, PlotStyle → Orange],
 ParametricPlot[{Re[w4[1 + I, τ]], Im[w4[1 + I, τ]]}, {τ, -60, 60},
  PlotRange → {{-0.4, 0.4}, {-0.1, 0.6}}, PlotStyle → Green],
 ParametricPlot[{Re[w5[1 + I, τ]], Im[w5[1 + I, τ]]}, {τ, -60, 60},
  PlotRange → {{-0.4, 0.4}, {-0.1, 0.6}}, PlotStyle → Purple]]
```

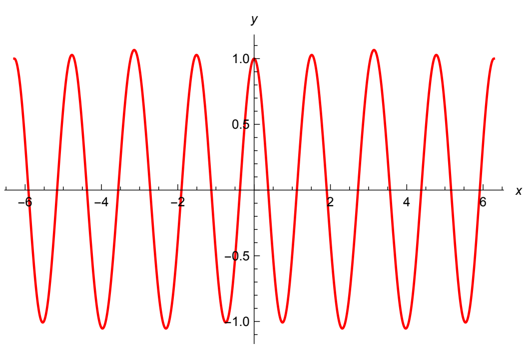


Appendix C. Real Fourier Series Solution (Mathieu Equation)

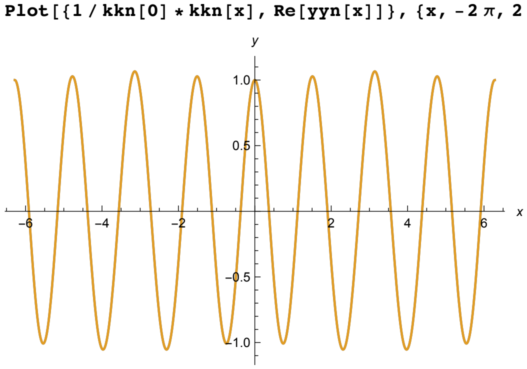
```
Clear["`*"]

(*Set the maximum value for evaluating the polynomials to*)
max = 20;

(*Define the infinite matrix, recalling that our true
 infinite matrix differs slightly to the Jacobi matrix*)
nn = DiagonalMatrix[Table[-k^2, {k, 0, max}]] +
   DiagonalMatrix[Table[1., {k, 0, max - 1}], 1] +
   DiagonalMatrix[Flatten[{2, Table[1., {k, 0, max - 2}]}], -1];

(*Obtain the eigenvalues and eigenvectors*)
{val, vec} = Eigensystem[nn];

(*Use the eigenvectors/orthogonal polynomials to compute the partial sum,
evaluated at some fixed eigenvalue*)
kkn[x_] := Sum[vec[[-5, j]] * Cos[(j - 1) * x], {j, 1, max}]

(*Plot this partial sum to see the shape of the output*)
Plot[kkn[x], {x, -2 π, 2 π}, AxesLabel → {x, y}, PlotStyle → Blue]
```




```
(*Numerically solve the Mathieu equation at some fixed
 eigenvalue using DSolve and appropriate initial conditions*)
yyn = DSolveValue[
   {y''[x] + 2 * Cos[x] * y[x] == val[[-5]] * y[x], y[0] == 1, y'[0] == 0}, y, x];

(*Plot the periodic solution of the Mathieu equation*)
Plot[Re[yyn[x]], {x, -2 π, 2 π}, AxesLabel → {x, y}, PlotStyle → Red]
```

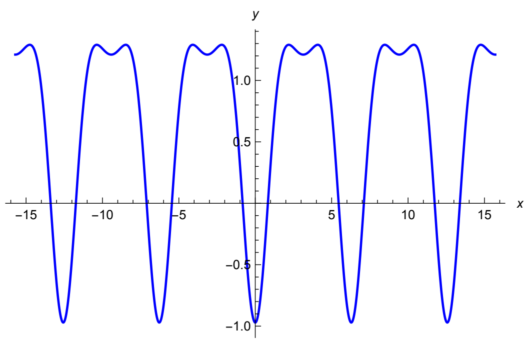



```
(*Overlay the discrete and continuous solutions for comparison, recalling
 that we need to multiply the partial sum by an appropriate constant*)
Plot[{1 / kkn[0] * kkn[x], Re[yyn[x]]}, {x, -2 π, 2 π}, AxesLabel → {x, y}]
```

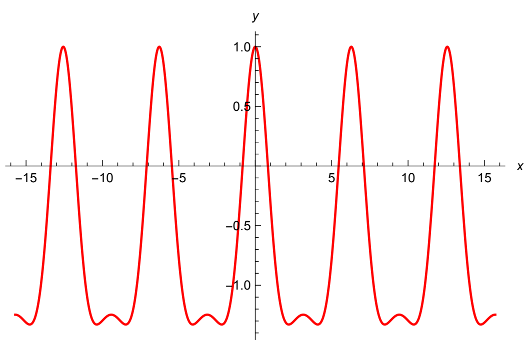


Appendix D. Complex Fourier Series Solution (Mathieu Equation)

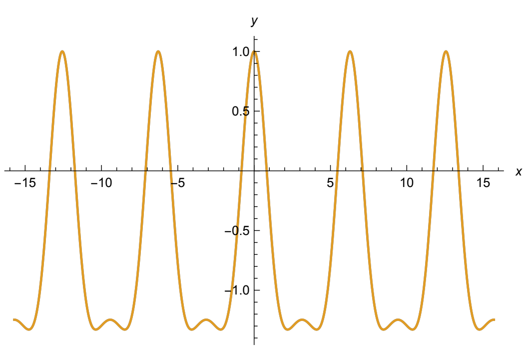
```
Clear["`*"]

(*Set the maximum value for evaluating the polynomials to*)
max = 40;

(*Define the infinite Jacobi matrix*)
mm = DiagonalMatrix[Table[-k^2, {k, -max, max}]] +
   DiagonalMatrix[Table[1., {k, -max, max - 1}], 1] +
   DiagonalMatrix[Table[1., {k, -max, max - 1}], -1];

(*Obtain the eigenvalues and eigenvectors*)
{val, vec} = Eigensystem[mm];

(*Use the eigenvectors/orthogonal polynomials to compute the partial sum,
evaluated at some fixed eigenvalue*)
kk[x_] := Sum[vec[[-3, j]] * Exp[I * (j - max - 1) x], {j, 1, 2 max + 1}];

(*Plot this partial sum to see the shape of the output*)
Plot[kk[x], {x, -5 π, 5 π}, PlotStyle → Blue, AxesLabel → {x, y}]
```




```
(*Numerically solve the Mathieu equation at some fixed eigenvalue
 using DSolve and appropriate initial conditions*)yy = DSolveValue[
   {y''[x] + 2 * Cos[x] * y[x] == val[[-3]] * y[x], y[0] == 1, y'[0] == 0}, y, x];

(*Plot the periodic solution of the Mathieu equation*)
Plot[yy[x], {x, -5 π, 5 π}, PlotStyle → Red, AxesLabel → {x, y}]
```




```
(*Overlay the discrete and continuous solutions for comparison, recalling
 that we need to multiply the partial sum by an appropriate constant*)
Plot[{(1 / kk[0]) * kk[x], yy[x]}, {x, -5 π, 5 π}, AxesLabel → {x, y}]
```



Appendix E. Connection to the Chebyshev Moment Problem

```
Clear["`*"]

(*Suppose that we know the solution to the Chebyshev moment problem,
σ(x), such that we can generate a positive sequence s_k*)

s[k_] := Integrate[x^k * 1 / Sqrt[1 - x^2], {x, -1, 1}];

Table[s[k], {k, 0, 8}]
```

$$\left\{\pi,\ 0,\ \frac{\pi}{2},\ 0,\ \frac{3\,\pi}{8},\ 0,\ \frac{5\,\pi}{16},\ 0,\ \frac{35\,\pi}{128}\right\}$$

```
(*We can check that s_k is indeed a positive sequence
 by checking that the Hankel determinants are all positive*)

det = Table[Det[Table[s[i + j], {i, 0, max}, {j, 0, max}]], {max, 1, 6}]
```

$$\left\{\frac{\pi^2}{2},\ \frac{\pi^3}{16},\ \frac{\pi^4}{512},\ \frac{\pi^5}{65\,536},\ \frac{\pi^6}{33\,554\,432},\ \frac{\pi^7}{68\,719\,476\,736}\right\}$$

```
(*We construct the Hankel matrix appended with powers of λ,
in order to define an arbitrary orthogonal polynomial of degree n*)

mat = Table[Append[Table[s[i + j], {i, 0, max - 1}, {j, 0, max}],
    Table[λ^i, {i, 0, max}]], {max, 1, 6}];

(*Using the determinantal definition,
we construct an arbitrary polynomial of degree n, recalling that P_0(λ)=1*)

P = Table[1 / (det[[i - 1]] * det[[i]]) * Det[mat[[i]]], {i, 2, 6}]
```

$$\left\{\frac{8\left(-1+2\,\lambda^2\right)}{\pi^3},\ \frac{64\left(-6\,\lambda+8\,\lambda^3\right)}{\pi^4},\ \frac{2048\left(4-32\,\lambda^2+32\,\lambda^4\right)}{\pi^5},\right.$$
$$\left.\frac{65\,536\left(160\,\lambda-640\,\lambda^3+512\,\lambda^5\right)}{\pi^6},\ \frac{8\,388\,608\left(-256+4608\,\lambda^2-12\,288\,\lambda^4+8192\,\lambda^6\right)}{\pi^7}\right\}$$

```
(*Now we define the coefficients of the finite difference equation,
using the functional of a product of two polynomials for a_k,
and a product of the Hankel determinants for b_k*)

a = Table[λ * P[[i]] * P[[i]] /. {λ → s[1], λ^2 → s[2], λ^3 → s[3],
    λ^4 → s[4], λ^5 → s[5], λ^6 → s[6], λ^7 → s[7], λ^8 → s[8]}, {i, 2, 5}]
```

{0, 0, 0, 0}

```
b = Table[Sqrt[det[[i - 1]] * det[[i + 1]]] / det[[i]], {i, 2, 5}]
```

$$\left\{\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right\}$$

```
(*This simply gives us the following infinite Jacobi matrix*)

mm =
  DiagonalMatrix[Table[0, {k, 0, 5}]] + DiagonalMatrix[Table[1 / 2, {k, 0, 4}], 1] +
   DiagonalMatrix[Table[1 / 2, {k, 0, 4}], -1];

mm // MatrixForm
```

$$\begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \end{pmatrix}$$