Spectral Theory of Orthogonal Polynomials

Barry Simon
IBM Professor of Mathematics and Theoretical Physics
California Institute of Technology
Pasadena, CA, U.S.A.

Lecture 7: Periodic OPRL
Spectral Theory of Orthogonal Polynomials

- Lecture 5: Killip–Simon Theorem on $[-2, 2]$
- Lecture 6: Szegő Asymptotics and Shohat-Nevai for $[-2, 2]$
- Lecture 7: Periodic OPRL
- Lecture 8: Finite Gap Isospectral Torus
References


The lecture title is a bit of a misnomer in that we’ll mainly discuss whole line periodic Jacobi matrices although the half-line objects will enter a lot in future lectures.

So \( \{a_n, b_n\}_{n=-\infty}^{\infty} \) are two-sided sequences with some \( p > 0 \) in \( \mathbb{Z} \) so that

\[
a_{n+p} = a_n \quad b_{n+p} = b_n
\]

For \( z \in \mathbb{C} \) fixed, we are interested in solutions \( \{u_n\}_{n=0}^{\infty} \) of

\[
a_n u_{n+1} + b_n u_n + a_{n-1} u_{n-1} = zu_n
\]
that also obey for some $\lambda \in \mathbb{C}$ ($\lambda = e^{i\theta}$, $\theta \in \mathbb{C}$)

\[ u_{n+p} = \lambda u_n \]

Such solutions are called Floquet solutions as they are analogs of solutions of ODE, especially Hill’s equation

\[-u'' + Vu = z u, \ V(x+p) = V(x).\]

The analysis of such solutions is a delightful amalgam of three tools, the first of which is just the fact that the set of all solutions of the difference equation is two-dimensional.

Thus, there are, for $z$ fixed, at most two different $\lambda$’s for which there is a solution. If $\lambda_1$, $\lambda_2$ are two such $\lambda$’s, their Wronskian is non-zero so constancy of the Wronskian implies $\lambda_1 \lambda_2 = 1$. 
The (twisted) periodic boundary condition Jacobi matrix $J^\text{per, } \lambda$ is $p \times p$. It is the finite Jacobi matrix with $1p$ and $p1$ matrix elements added:

$$J_{jj} = b_j, \quad J_{j \, j+1} = a_j, \quad J_{j \, j-1} = a_{j-1}$$

$$J_{1p} = a_p \lambda^{-1}, \quad J_{p1} = a_p \lambda$$

If $\{u_n\}_{n=-\infty}^{\infty}$ is a Floquet solution, $u_0 = \lambda^{-1} u_p$, $u_{p+1} = \lambda u_1$ so $\tilde{u} = \{u_n\}_{n=1}^{p}$ has $J^\text{per, } \lambda \tilde{u} = z \tilde{u}$.

Conversely, if $\tilde{u}$ solves this, the unique $u$ with $u_{n+p} = \lambda u_n$ and $\tilde{u} = \{u_n\}_{n=1}^{\infty}$ is a Floquet solution.
This implies

- For any $\lambda$, there are at most $p$ $z$’s which have a Floquet solution for that $\lambda$. (We’ll see soon that if $\lambda \neq \pm 1$, there are exactly $p$.)

- If $\lambda = e^{i\theta}$, $\theta \in \mathbb{R}$, $\lambda \neq \pm 1$, there are precisely $p$ distinct $z$’s all real, for which there are Floquet solutions with that $\lambda$.

The reality comes from hermicity of $J_{\text{per},\lambda}$.

If $\lambda \neq \pm 1$, $\bar{\lambda} \neq \lambda$. If $u$ is a Floquet solution for $\lambda$, since $z$ is real, $\bar{u}$ is a Floquet solution for $\bar{\lambda}$ so there is a unique solution for that $z$. Thus, for $\lambda \in \partial \mathbb{D} \setminus \{\pm 1\}$, $J_{\text{per},\lambda}$ has $p$ eigenvalues and each simple.
The third tool concerns the $p$-step transfer matrix.

$$T_p(z)\left(\begin{array}{c} u_1 \\ a_0 u_0 \end{array}\right) = \lambda \left(\begin{array}{c} u_1 \\ a_0 u_0 \end{array}\right)$$ is equivalent to \( \left(\begin{array}{c} u_1 \\ a_0 u_0 \end{array}\right) \) generating a Floquet solution! (Note: \(a_0\) may not be 1.)

In terms of the OP’s for \(\{a_n, b_n\}_{n=1}^\infty\),

$$T_p(z) = \left(\begin{array}{cc} p_p(z) & -q_p(z) \\ a_p p_{p-1}(z) & -a_p q_{p-1}(z) \end{array}\right)$$

The discriminant, \(\Delta(z)\), is defined by

$$\Delta(z) = \text{Tr} \left( T_p(z) \right) = p_p(z) - a_p q_{p-1}(z)$$

is a (real) polynomial of degree exactly \(p\).
Since \( \det(T_p(z)) = 1 \), it has algebraic eigenvalues \( \lambda \) and \( \lambda^{-1} \) where

\[
\Delta(z) = \lambda + \lambda^{-1}; \quad \Delta(z) = 2 \cos \theta \text{ if } \lambda = e^{i\theta}.
\]

Floquet solutions correspond to geometric eigenvalues for \( T_p(z) \). If \( \lambda \neq \pm 1 \), it has multiplicity one, so is geometric. \( \lambda = \pm 1 \) has multiplicity 2, so there can be one or two Floquet solutions.

An important consequence of the fact that \( \Delta(z) \in (-2, 2) \) implies all \( z \)'s are real is \( \Delta^{-1}[(-2, 2)] \subset \mathbb{R} \).
A basic fact of analytic functions is that if $f(z)$ is real (i.e., $f(\bar{z}) = f(z)$), $x_0 \in \mathbb{R}$ with $f'(x_0) = 0$, there are non-real $z$’s near $x_0$ with $f(z)$ real and near $f(x_0)$.

Thus, $\Delta^{-1}[-2, 2] \subset \mathbb{R} \Rightarrow \Delta'(x_0) \neq 0$ if $\Delta(x_0) \in (-2, 2)$.

Thus, $\Delta^{-1}[-2, 2] = (\alpha_1, \beta_1) \cup (\alpha_2, \beta_2) \cup \ldots \cup (\alpha_p, \beta_p)$

where $\alpha_1 < \beta_1 \leq \alpha_2 < \beta_2 \leq \alpha_3 < \ldots < \beta_p$

with $\Delta$ a smooth bijection of $(\alpha_j, \beta_j)$ to $(-2, 2)$.

Could be orientation reversing or not.
The Discriminant

Since $\Delta(x) \to \infty$ as $x \to \infty$, we must have $\Delta(\beta_p) = 2$.

It follows that $\Delta(\alpha_p) = -2$, $\Delta(\beta_{p-1}) = -2$, $\Delta(\alpha_{p-1}) = 2 \ldots$

i.e., $\Delta(\beta_j) = (-1)^{p-j}2$, $\Delta(\alpha_j) = (-1)^{p-j-1}2$

If the $\alpha$’s and $\beta$’s are all distinct, we have $p$ points where $\Delta(x) = 2$ and $p$ where $\Delta(x) = -2$.

Since $\deg \Delta = p$, these are all the points.

If $\beta_{j-1} = \alpha_j$, there is one less point where $\Delta(x) = (-1)^{p-j-1}2$, but $\Delta'(\alpha_j) = 0$ since $\Delta - (-1)^{p-j-1}2$ has the same sign on both sides of $\alpha_j$. It follows that
Theorem. $\Delta^{-1}([-2, 2]) = \bigcup_{j=1}^{p} [\alpha_j, \beta_j]$ and

$\Delta^{-1}([-2, 2]) = \{\alpha_j, \beta_j\}_{j=1}^{p}$ and

$\Delta'(\alpha_j) = 0 \iff \alpha_j = \beta_{j-1}$, $\Delta'(\beta_j) = 0 \iff \beta_j = \alpha_{j+1}$

and in that case, $\Delta''$ is not zero at that point.

The $[\alpha_j, \beta_j]$ are called the bands and $(\beta_j, \alpha_{j+1})$ the gaps.

If $\beta_j < \alpha_{j+1}$, we say that gap $j$ is open.

If $\beta_j = \alpha_{j+1}$, we say gap $j$ is closed.
Furthur analysis shows at a closed gap (with $\Delta(\alpha) = 2$ for simplicity) there are two periodic (Floquet) solutions, while at each of the edges of an open gap there is only one periodic (Floquet) solution. The transfer matrix has a Jordan anomaly, i.e., $\det = 1$, $\Tr = 2$, but $T \neq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

Each of the gaps where $\Delta(x) \geq 2$ has two periodic solutions—either two at $\beta_j = \alpha_{j+1}$ or one each at $\beta_j$ and $\alpha_{j+1}$ so there are $p$ periodic Floquet solutions, as there must be from the $J_{\text{per}}$ analysis.
Spectrum and Spectral Types

If \( z \) is such that \( \Delta(z) \not\in [-2, 2] \), then the roots of \( \lambda + \lambda^{-1} = \Delta(z) \) have \( |\lambda| > 1, |\lambda^{-1}| < 1 \). It follows that there are different solutions \( u_\pm \) decaying exponentially at \( \pm\infty \) so their Wronskian is not zero. By the earlier analysis,

\[
G_{nm}(z) = u_{\max(n,m)}^+(z) u_{\min(m.n)}^-(z)/W(z)
\]

is the matrix for \((J - z)^{-1}\), i.e., \( z \notin \sigma(J) \).

If \( \Delta(z) \in [-2, 2] \), there is a bounded Floquet solution (since \( |\lambda| = 1 \)). Then \( \| (J - z)[u \chi_{[-N,N]}] \| \) is bounded, but since \( \sum_{j=1}^{p} |u_{m+j}|^2 \) is constant, \( \| u \chi_{[-N,N]} \| \to \infty \) so \( z \in \sigma(J) \). Thus

**Theorem.** \( \sigma(J) = \bigcup_{j=1}^{p} [\alpha_j, \beta_j] \).
If $\Delta(z) \in (-2, 2)$, we get that all solutions are bounded at $\pm \infty$ and then by a Wronskian argument, $|u_n|^2 + |u_{n+1}|^2$ is bounded from below. So by a Carmona-type formula, one should expect purely a.c. spectrum. But this is whole line, not half line!

Here is a replacement: Away from the bands, $G_{nn} = u_n^+ u_n^- / W$ as we’ve seen. By continuity of eigenfunctions of transfer matrix in $z$, $u_n^\pm$ has a limit at $z = x + i \varepsilon$ with $\varepsilon \downarrow 0$ which are Floquet solutions. This is true at least at interiors of bands where the transfer matrix has distinct eigenvalues.
$W$ is non-vanishing on each $(\alpha_j, \beta_j)$ since $u^+$ and $u^-$ are distinct Floquet solutions $(e^{\pm i\theta})$. Thus, $G_{nn}(z)$ is continuous from $\mathbb{C}_+$ to $\mathbb{C}_+ \cup \mathbb{R} \setminus \{\alpha_j, \beta_j\}_{j=1}^p$.

But if $\mu^{(n)}$ is the spectral measure of $\delta_n$:

$$G_{nn}(z) = \int \frac{d\mu^{(n)}(x)}{x - z}$$

The continuity implies $d\mu^{(n)}$ is purely a.c., so we have proven

**Theorem.** A periodic two-sided Jacobi matrix has purely absolutely continuous spectrum.

One can write out an explicit spectral representation with Floquet solutions with $z \in (\alpha_j, \beta_j)$ as continuum eigenfunctions.
We start with a puzzle. \( \Delta \) determines 
\( \alpha_1 < \beta_1 \leq \alpha_2 < \beta_2 \leq \ldots \) as the roots of \( \Delta^2 - 4 \).

Conversely, given \( \beta_p, \alpha_{p-1}, \beta_{p-2}, \ldots, \Delta - 2 \) is determined up to a constant since we know its zeros.

That constant is determined by \( \alpha_p \) when \( \Delta \) is \( -2 \). Thus, \( \beta_p, \alpha_{p-1}, \beta_{p-2} \) plus \( \alpha_p \) determine the remaining \( p - 1 \) \( \alpha \)'s and \( \beta \)'s. Why this rigidity? Why can’t we have \( 2p \) arbitrary \( \alpha \)'s and \( \beta \)'s?

The answer will lie in potential theory.
For any $z \in \mathbb{C}$, there are two Floquet indices, $\lambda_{\pm}$, solving $\lambda + \lambda^{-1} = \Delta(z)$. If $|\lambda_+| \geq 1$, we see that

$$\gamma(z) = \lim_{n \to \infty} \frac{1}{n} \log \|T_n(\lambda)\| = \frac{1}{p} \log |\lambda_+(z)|$$

Solving the quadratic equation for $\lambda$

$$\gamma(z) = \frac{1}{p} \left[ \log \left| \frac{\Delta(z)}{2} + \sqrt{\left( \frac{\Delta(z)}{2} \right)^2 - 1} \right| \right]$$

On $\varepsilon = \bigcup_{j=1}^{p} [\alpha_j, \beta_j], |\ldots| = 1$, so $\gamma(z) \geq 0$, $\gamma(z) = 0$ on $\varepsilon$. $\gamma(z)$ is harmonic on $\mathbb{C} \setminus \varepsilon$

since $\frac{\Delta}{2} + \sqrt{(\frac{\Delta}{2}) - 1}$ is analytic and non-vanishing there and $\gamma(z) = \log (|z|) + O(1)$ at $\infty$, since $\Delta(z)$ is a degree $p$ polynomial.
Thus $\gamma(z) = G_e(z)$ is the potential theorists’ Green’s function. Thus,

**Theorem.** $\gamma(z)$ as given above is the potential theorists’ Green’s function and periodic Jacobi parameters are associated to regular measures (in the Stahl–Totik sense).

**Corollary.** $C(e) = (a_1 \cdots a_p)^{1/p}$
By general principles, if $G_\epsilon$ is smooth up to $\epsilon$ on $\epsilon^{\text{int}}$, the equilibrium measure $d\rho_\epsilon(x) = f_\epsilon(x)dx$ where

$$f_\epsilon(x) = \frac{1}{\pi} \frac{\partial}{\partial y} G_\epsilon(x + iy) \mid_{y=0}$$

Thus, the equilibrium measure is

$$f_\epsilon(z) = \frac{1}{p\pi} \frac{|\Delta'(x)|}{\sqrt{4 - \Delta^2(x)}} = \frac{1}{p\pi} \left| \frac{d}{dx} \arccos\left(\frac{\Delta(x)}{2}\right) \right|$$
In each, band $\Delta(\lambda)$ goes from $-2$ to $2$, so $\arccos(\frac{\Delta}{2})$ from $\pi$ to $0$. Thus,

**Theorem.** $\rho_\epsilon([\alpha_j, \beta_j]) = \frac{1}{p}$.

This explains the puzzle mentioned earlier.

This is also a density of zeros way of understanding why the above $f_\epsilon$ is the DOS. For the periodic eigenfunctions with a box of size $kp$ are the Floquet solutions with $\lambda = e^{2\pi ij/k}$, $j = 0, 1, 2, \ldots, k - 1$. 