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A useful formula for periodic Jacobi matrices on trees

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We introduce a function of the density of states for periodic Jacobi matrices on trees and prove a useful formula for it in terms of entries of the resolvent of the matrix and its "half-tree" restrictions. This formula is closely related to the one-dimensional Thouless formula and associates a natural phase with points in the bands. This allows streamlined proofs of the gap labeling and Aomoto index theorems. We give a complete proof of gap labeling and sketch the proof of the Aomoto index theorem. We also prove a version of this formula for the Anderson model on trees.

Jacobi matrices | trees | spectral theory

Significance

The subject of periodic Jacobi matrices on trees has evoked interest among mathematical physicists, analysts, and number theorists. We introduce a function of use in the study of these objects and prove a useful formula for this function. We illustrate the usefulness of this formula by using it to provide a proof of gap labeling that does not use C^*-algebras. We also use it to provide an understanding of the Aomoto index theorem.

1. Introduction

Graph Jacobi matrices provide a unified framework for dealing with graph adjacency matrices, weighted Laplacians, and Schrödinger operators. Their spectral theory therefore has connections with various fields, among those are mathematical physics, analysis, probability, and number theory. This note deals with periodic Jacobi matrices on trees, which arise through viewing the tree as the universal cover of a finite graph. Such operators have attracted a considerable amount of interest recently (1–15). The purpose of this note is to announce and give an interim report on the use of a formula which, in particular, provides a short proof of Sunada's gap labeling result (14), without the use of C^* algebras.

We start with a connected, finite graph, $\mathcal{G}$, which can have self-loops and multiple edges between a pair of vertices but which, for simplicity of exposition, we suppose is leafless. We use $V(\mathcal{G})$ for the vertex set of $\mathcal{G}$ and $E(\mathcal{G})$ (sometimes just V and E) for the set of edges. We pick an orientation for each edge, e, using $\check{e}$ for the oppositely directed edge. $\sigma(e)$ is the initial vertex and $\tau(e)$ the final of the directed edge e, so for example, $\sigma(\check{e}) = \tau(e)$. We let $\tilde{E}$ denote the set of all edges with arbitrary assigned orientation so that $\#(\tilde{E}) = 2\#(E)$. We assign a potential, $b(v) \in \mathbb{R}$, to each vertex and coupling, $a(e) = a(\check{e}) > 0$, to each edge, calling these the *Jacobi parameters* of $\mathcal{G}$.

Let $\mathcal{T}$ be the universal cover of $\mathcal{G}$—it is always an infinite tree, and let $\pi : \mathcal{T} \to \mathcal{G}$ be the covering map. We can lift the Jacobi parameters of $\mathcal{G}$ to $\mathcal{T}$ by setting $b(\tilde{v}) = b(\pi(\tilde{v}))$; $\quad a(\tilde{e}) = a(\pi(\tilde{e}))$. One defines an infinite matrix, H, indexed by $V(\mathcal{T})$ by

$$H_{\tilde{v}\tilde{w}} = \begin{cases} b(\tilde{v}), & \text{if } \tilde{v} = \tilde{w} \\ a(\tilde{e}), & \text{if } (\tilde{v}\tilde{w}) = \tilde{e} \text{ an edge in } \tilde{E}(\mathcal{T}) \\ 0, & \text{otherwise} \end{cases} \quad \textbf{[1]}$$

and a corresponding bounded self-adjoint operator, H, on $\mathcal{H} = \ell^2(V(\mathcal{T}))$. One defines the *period*, p, to be $\#(V(\mathcal{G}))$. If $\mathcal{G}$ is a single cycle, then $\mathcal{T}$ is $\mathbb{Z}$ and the Jacobi parameters are periodic in the naive sense. This classical subject (of $1D$ periodic Jacobi matrices) has been extensively studied; see for example, Simon (16, Chaps. 5, 6, 8).

Deck transformations induce unitary maps on $\mathcal{H}$ which commute with H. In particular, for every $v \in V(\mathcal{G})$, the spectral measure, $d\mu_{\tilde{v}}$, and Green's function, $\langle \delta_{\tilde{v}}, (H-z)^{-1}\delta_{\tilde{v}} \rangle$, are the same for all $\tilde{v} \in V(\mathcal{T})$ with $\pi(\tilde{v}) = v$. We use $d\mu_v$ and $G_v(z)$ for these common values. It is a basic fact that in one form goes back at least to ref. 17 (see also refs. 11 and 18) that each $G_v(z)$ defined for $z \in \mathbb{C}_+$ is an algebraic function which can be continued across the real axis with finitely many points removed (this implies, see ref. 4, *Theorem* 6.7, that the spectrum of H has no singular continuous part and the densities of the a.c. part of the spectral measures are real analytic in the interior of the spectrum except for possible algebraic singularities).

One defines the *density of states* measure, $dk(E)$ (and *integrated density of states*, aka IDS, $k(E) = dk((-\infty, E))$), by

$$dk = \frac{1}{p} \sum_{v \in V} d\mu_v \quad \textbf{[2]}$$

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Remark For Jacobi matrices on $\mathbb{Z}^\nu$, the analog is the limiting empirical spectral distribution of the Jacobi matrices associated with larger and larger boxes (with, say, free boundary conditions); because truncated trees have so many boundary points, the same is not true for trees with general boundary conditions (BC) although one can carefully choose periodic BC so that it is (3).

The support of the measure dk is the spectrum of H and by the definition of spectral measures, one has that

$$\int \frac{1}{\lambda - z}\, dk(\lambda) = \frac{1}{p} \sum_{v \in V} G_v(z) \qquad [3]$$

One of the fundamental results of the theory is as follows:

Theorem 1. *[Sunada (14)] In any gap of the spectrum of H, the IDS is an integral multiple of $1/p$. In particular, the spectrum has at most p connected components.*

Sunada's proof, while elegant, is involved since it uses some deep results of Pimsner–Voiculescu (19) from the K-theory of C^*-algebras. One of our main results is a short proof of Sunada's theorem that, in particular, makes no use of C^*-algebras.

Another fundamental result is the Aomoto index theorem. In the $1D$ case, H does not have any point spectrum but in other cases that is not true—see, for example, Avni et al. (4, Example 7.2) or the extensive study in Banks et al. (5). In that case, given an eigenvalue, λ, define $X_1(\lambda)$ to be the set of vertices, $v \in V$, so that for some $\tilde{v}$ with $\pi(\tilde{v}) = v$ there is some eigenfunction ψ associated to λ, with $\psi(\tilde{v}) \neq 0$. Define $\partial X_1(\lambda)$ to be those $v \in V$ not in $X_1(\lambda)$ but neighbors of points in $X_1(\lambda)$, and we let $E(\lambda)$ be the set of edges with both endpoints in $X_1(\lambda)$.

Theorem 2. *[Aomoto Index Theorem (2)] The measure dk has a mass at an eigenvalue, λ, of weight $I(\lambda)/p$ where*

$$I(\lambda) = \#(X_1(\lambda)) - \#(\partial X_1(\lambda)) - \#(E(\lambda)) \qquad [4]$$

A second proof of this theorem can be found in Banks et al. (5). Both earlier proofs involve detailed combinatorial analyses. The second of our results here is a different proof of the Aomoto index theorem that some may find simpler but that, in any event, is very illuminating.

Our approach concerns a basic function which we will call the *Floquet function* defined in $\mathbb{C}_+$ by

$$\Phi(z) = \exp\left(p \int \log(t - z)\, dk(t)\right) \qquad [5]$$

which clearly has an analytic continuation to a neighborhood of $\mathbb{C}_+ \cup (\mathbb{R} \setminus \mathrm{spec}(H))$. In the $1D$ case, under the normalization $\prod_{j=1}^{p} a_j = 1$, the Thouless formula (16, *Theorem* 5.4.12) implies that if $u_j(z)$ is a *Floquet solution* (i.e., solution of the difference equation

$$a_j u_{j+1} + b_j u_j + a_{j-1} u_{j-1} = z u_j \qquad [6]$$

with $u_{j+p} = A u_j$ for a constant A), then (16, *Theorem* 5.4.15) $(-1)^p A = \Phi(z)$ or $\Phi(z)^{-1}$ which is why we give Φ this name. There is another approach to 1D periodic Jacobi matrices that extends the celebrated work of Marchenko–Ostrovskii (20) from the case of Hill's ODE (a pedagogical discussion of the 1D periodic Jacobi matrix Marchenko–Ostrovskii theory can be found in Lukic [21, esp. (10.47) and (10.48)]. The Marchenko–Ostrovskii conformal map is (up to a factor of i and unimportant constant), the logarithmic integral appearing in (1.5). So our Floquet function can also be viewed as an extension of the Marchenko–Ostrovskii conformal map from cyclic graphs to general finite graphs.

Because of Eq. **3** we have that

$$\frac{d}{dz} \log(\Phi(z)) = -\sum_{v \in V} G_v(z) \qquad [7]$$

In Section 2, we will prove an explicit formula for the Floquet function in terms of Green's functions and m-functions (objects whose definition we recall there). In Section 3, we will use this Floquet formula to prove the Sunada gap labeling theorem and in Section 4, we will sketch our proof of the Aomoto index theorem (in the case where the eigenvalue is isolated from the continuous spectrum; see the discussion there). In Section 5, we will discuss a version of the Floquet formula for the Anderson model on trees. Since, as we will explain, one can regard the Floquet formula as half a Thouless formula, we hope to find some interesting applications of that result.

2. The Floquet Formula

We will prove a useful formula for the Floquet function. To do so, we need to recall what the m-functions are and the relations between the Green's and m-functions. Given $e \in E$, pick $\tilde{e} \in E(\mathcal{T})$ with $\pi(\tilde{e}) = e$. Removing $\tilde{e}$ from $\mathcal{T}$ breaks that graph into two pieces, $\mathcal{T}_{\tilde{e}}^{+}$ with $\tau(\tilde{e})$ and $\mathcal{T}_{\tilde{e}}^{-}$ with $\sigma(\tilde{e})$. We let $H_{\tilde{e}}^{\pm}$ be the operators on $\ell^2(V(\mathcal{T}_{\tilde{e}}^{\pm}))$ with the restricted Jacobi parameters and set

$$m_e(z) = \langle \delta_{\tau(\tilde{e})}, (H_{\tilde{e}}^{+} - z)^{-1} \delta_{\tau(\tilde{e})} \rangle \qquad [8]$$

The use of deck transformations shows this depends only on e and not the choice of $\tilde{e}$ over e.

The use of the method of Schur complements (see ref. 4, Section 6 for a proof; the formulae appear at least as early as ref. 22, Proposition 2.1) shows that

$$\frac{1}{G_u(z)} = -z + b_u - \sum_{f \in \tilde{E}:\, \sigma(f) = u} a_f^2 m_f(z) \qquad [9]$$

$$\frac{1}{m_f(z)} = -z + b_u - \sum_{\substack{f' \in \tilde{E}, f' \neq \check{f} \\ \sigma(f') = \tau(f)}} a_{f'}^2 m_{f'}(z) \qquad [10]$$

which implies for any $e \in \tilde{E}$ that

$$G_{\sigma(e)} = \frac{1}{m_{\check{e}}^{-1} - a_e^2 m_e} = \frac{m_{\check{e}}}{1 - a_e^2 m_e m_{\check{e}}} \qquad [11]$$

Define

$$Q_e(z) = \frac{1}{1 - a_e^2 m_e(z) m_{\check{e}}(z)} = \frac{G_{\sigma(e)}(z)}{m_{\check{e}}(z)} = \frac{G_{\tau(e)}(z)}{m_e(z)} \qquad [12]$$

We are heading toward the proof of a lovely formula we call the *Floquet formula*:

Theorem 3. *[Floquet Formula] We have that*

$$\Phi(z) = \frac{\prod_{e \in E(\mathcal{G})} Q_e(z)}{\prod_{u \in V(\mathcal{G})} G_u(z)} \qquad [13]$$

initially for $z \in \mathbb{C}_+$, but the right side defines a meromorphic continuation to $(\mathbb{C} \setminus \mathrm{spec}(H)) \cup ($*isolated point spectrum of* $H)$.

Remark Using Eq. **12**, this can also be written

$$\Phi(z) = \frac{\prod_{e\in E(\mathcal{G})} G_{\tau(e)}(z)}{\prod_{u\in V(\mathcal{G})} G_u(z) \prod_{e\in E(\mathcal{G})} m_e(z)} \quad \textbf{[14]}$$

In particular, this implies that Φ is an algebraic function.

We sketch our proof of this result. Let Ψ be the right side of Eq. **13**. It is easy to see that as $x \to \infty$ in $\mathbb{R}$, that $\Phi(-x) = x^p + O(x^{p-1})$ and $\Psi(-x) = x^p + O(x^{p-1})$ so to prove Eq. **13**, it suffices to prove that for $z \in \mathbb{C}_+$

$$\log(\Psi)'(z) = \log(\Phi)'(z) \quad \textbf{[15]}$$

where $\cdot' = \frac{d\cdot}{dz}$.

To compute $\log(\Psi)'(z)$, we note that, by Eq. **9**, we have that

$$\begin{aligned}(\log(G_u))' &= -\left(\log\left(\frac{1}{G_u}\right)\right)' = -G_u\left(\frac{1}{G_u}\right)' \\ &= G_u + \sum_{e\in\tilde{E}:\ \sigma(e)=u} a_e^2 m_e' G_u \end{aligned} \quad \textbf{[16]}$$

and that by, Eq. **12**,

$$\begin{aligned}(\log(Q_e))' &= (a_e^2 m_e' m_{\tilde{e}} + a_e^2 m_e m_{\tilde{e}}')Q_e \\ &= a_e^2 G_{\sigma(e)} m_e' + a_e^2 G_{\tau(e)} m_{\tilde{e}}' \end{aligned} \quad \textbf{[17]}$$

Therefore

$$\begin{aligned}\sum_{e\in E}(\log(Q_e))' &= \sum_{e\in\tilde{E}} a_e^2 G_{\sigma(e)} m_e' \\ &= \sum_{u\in V} \sum_{e\in\tilde{E}:\ \sigma(e)=u} a_e^2 m_e' G_u \\ &= \sum_{u\in V}(-G_u + (\log(G_u))') \end{aligned} \quad \textbf{[18]}$$

which, by Eq. **7**, proves Eq. **15** and so *Theorem* 3.

3. Gap Labeling

In this section, we present our proof of Sunada's Gap Labeling theorem, *Theorem* 1. Basically, it is an immediate consequence of the Floquet formula Eq. **13**. We need some care in determining the branch of log used Eq. **5**. We pick the branch where when $z \in \mathbb{C}_+$ is taken near $-\infty$ on the real axis, Φ has an argument near 0. That is, we are using the branch where when $z = -x$ (x near $+\infty$) and t in a bounded interval, we have that $\log(t - z) > 0$ and we are then continuing z through the upper plane. Thus, if E_0 is a real point in the resolvent set of H, the integral defining Φ, Eq. **5**, can be analytically continued from $\mathbb{C}_+$ to a neighborhood of E_0 and for $s = t - E_0 \neq 0$ real, we have that

$$\mathrm{Im}(\log(s)) = \begin{cases} 0, & \text{if } s > 0 \\ -\pi, & \text{if } s < 0 \end{cases} \quad \textbf{[19]}$$

Moreover, the Floquet formula can be analytically continued to a set including E_0. Thus

$$\mathrm{Im}\left(p\int \log(t - E_0)\, dk(t)\right) = -p\pi k(E_0) \quad \textbf{[20]}$$

That means that $pk(E_0) \in \mathbb{Z} \iff \Phi(E_0)$ is real. But for $x \in \mathbb{R} \setminus \mathrm{spec}(H)$, each $G_v(x)$ and $m_e(x)$ is analytic (meromorphic for m), we see that except for potential isolated poles (actually, it is easy to see that Φ has no poles), Φ is real in gaps!

4. Aomoto Index Theorem

In this section, we will sketch (with full details in a later publication) a proof of the Aomoto Index Theorem (*Theorem* 2) at least in the case where the eigenvalue is an isolated point of the spectrum (we hope in the later publication to deal with the general case; we will explain the potential difficulty soon—see point (1) below; the next paragraph also uses that the eigenvalue is isolated). We note that the earlier proofs of this theorem (2, 5) handle the general case and that Banks et al. (5) provide examples where there are nonisolated eigenvalues and also where there are isolated eigenvalues.

The Floquet function is involved with the question of the weight of an eigenvalue because, by the discussion in the last section, λ is an isolated eigenvalue with dk-weight I/p if and only if the argument of $\Phi(x)$ jumps by $I\pi$ as x passes through λ. For isolated eigenvalues, by the Sunada *Theorem*, I is an integer so this happens if and only if Φ has a zero of order I at λ.

The punch line is that Eq. **4** will come from the Floquet formula, Eq. **13**, and the fact that $G_v(z)$ has a simple pole at $z = \lambda$ if and only if $v \in X_1(\lambda)$, it has a simple zero when $v \in \partial X_1(\lambda)$ and $Q_e(z)$ has a simple pole at $z = \lambda$ if and only if $e \in E(\lambda)$. There can be some additional zeros of G_v and Q_e but we will see that they cancel.

We will use $X_0(\lambda) = V \setminus (X_1(\lambda) \cup \partial X_1(\lambda))$. Henceforth, without loss, we can suppose that $\lambda = 0$ for simplicity of notation and we drop (λ) from $X_{0,1}(\lambda)$.

The proof relies on a sequence of observations:

(1) If 0 is an isolated point in the spectrum then all Green's and m-functions are meromorphic in a neighborhood of 0. If they have poles they are simple with negative residue and if they are zero, the zeros are simple with positive derivative (this follows from the fact that by the spectral theorem, the derivative of Green's and m-functions away from poles are strictly positive). Thus in counting the order of a zero in Eq. **14**, each G or m contributes either a single $+1$, -1, or 0. (For nonisolated zeros, the functions are only algebraic and so have Laurent–Puiseux series—one needs to track potential fractional powers; this is why we have limited our discussion here to isolated points of the spectrum).

(2) If $v \in X_1$, G_v has a simple pole at 0 and for other v's either a zero or a nonzero finite value at 0.

(3) A direct analysis of the possibilities proves that if $e = (vw)$ with both points in X_1, then m_e has a finite nonzero value at 0 so, by Eq. **12**, Q_e has a simple pole.

(4) A direct analysis of the possibilities proves that if $e = (vw)$ with $v \in X_1$, $w \in \partial X_1$, then $m_e(0) = 0$ and $m_{\tilde{e}}$ has a pole at 0 so Q_e has a finite, nonzero value at 0 (since $m_e m_{\tilde{e}}$ has a negative value at 0 so the denominator in the first equality in Eq. **12** is nonvarnishing) and $G_w(0) = 0$.

(5) A direct analysis of the possibilities proves that if $e = (vw)$ with both points not in X_1, then Q_e does not have a pole at 0 so by (3) and (4), Q_e has a pole at zero if and only if both endpoints lie in X_1.

(6) The final equalities in Eq. **12** show that if $e = (vw)$ and $Q_e(0) = 0$, then neither v nor w can lie in X_1. It also shows that if m_e has a pole at 0, and neither v nor w lies in X_1, then $Q_e(0) = 0$. It follows that for such e's, Q_e has a double 0 at 0 if both m_e and $m_{\tilde{e}}$ have poles there (by the first equality in

Eq. **12**), and Q_e has a simple pole at 0 if exactly one of them has a pole. Thus for such e's, we can count poles of m_e rather than zeros of Q_e so long as we run e through all of $\tilde{E}$.

(7) It follows from Eq. **9**, that if $G_u(0) = 0$, then at least one m_f with $u = \sigma(f)$ has a pole, and because poles all have negative residues, the converse is true. A careful analysis shows that if m_f with $\sigma(f) = u$ has a pole, then for any $e \neq f$ with $\sigma(e) = u$ and with $\tau(e) \notin X_1$, one can conclude that m_e is not infinite. This means if that there is a $1-1$ correspondence between $v \in X_0$ with $G_v(0) = 0$ and those e with m_e having a pole with $\sigma(e) \in X_0$. By the argument in (5), it also says that if $\sigma(e) \in \partial X_1$, $\tau(e) \notin X_1$, then m_e does not have a pole. These two conclusions show that the number of zeros of the $G_u(z)$ with $u \in X_0$ exactly cancels the number of zeros of $Q_e(z)$, for those e with no ends in X_1.

In summary, Theorem 3 allows us to compute the multiplicity of the zero of the Floquet function at any given point by counting the multiplicities of the zeroes and poles of the G_v and Q_e (keeping in mind that the Q_e are in the numerator and the G_v in the denominator). Specifically, point (2) shows that for each $v \in X_1(\lambda)$ the $G_v(z)$ has a simple pole at $z = \lambda$, which is responsible for the $\#(X_1(\lambda))$ in Aomoto's index formula. Point (3) shows that $Q_e(z)$ has a simple pole at $z = \lambda$ for all $e \in E(\lambda)$, which yields the $-\#(E(\lambda))$ in the index formula. And, point (4) shows that $G_v(z)$ has a zero for all $v \in \partial X_1(\lambda)$, yielding the $-\#(\partial X_1(\lambda))$ in the index formula. The other points argue that the other terms in the Floquet formula either do not contribute with a pole or a zero, or their contributions cancel out with each other.

We remark that the earlier proofs of Aomoto's theorem (2, 5) show that X_1 is a forest (disjoint union of trees) which allows one to prove that the index is also equal to $ccX_1(\lambda) - \#(\partial X_1(\lambda))$ where $ccX_1(\lambda)$ is the number of connected components of $X_1(\lambda)$. So long as we use the formula Eq. **4**, we do not need to prove the forest result.

5. Anderson Model on a Tree

In this final section, we will note that the ideas of Section 2 also imply results for the Anderson model on a tree, a subject with considerable work in both the physics (23–25) and mathematical physics (22, 26–29) literatures. One fixes a strictly positive integer, d, and considers a Jacobi matrix on the homogeneous tree of degree d. The a's and b's are both given by independent identically distributed (separately for a and b) random variables (for technical simplicity, we suppose the supports of the distributions are bounded). Most commonly the distributions of the a's set them to be identically one but that does not affect anything in our arguments.

For us, as for Klein (22), the density of states is given by the expectation of the spectral measure over the ensemble of random Hamiltonians. By taking expectations of Eqs. **7** and **18**, we prove that

$$\int \log(t-z)\,dk(t) = \left(\tfrac{d}{2} - 1\right)\mathbb{E}(\log(G_u)) - \tfrac{d}{2}\mathbb{E}(\log(m_e)) \qquad [21]$$

In case $d = 2$ this is what follows from the Thouless formula and (30, 1.7) so this is sort of a half-Thouless formula. We are currently studying possible applications of Eq. **21**.

Data, Materials, and Software Availability. There are no data underlying this work.

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