Spectral Theory and Spectral Gaps for Periodic Schrödinger Operators on Product Graphs

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Abstract

Floquet theory and its applications to spectral theory are developed for periodic Schrödinger operators on product graphs $\mathbb{G} \times \mathbb{Z}$, where $\mathbb{G}$ is a finite graph. The resolvent and the spectrum have detailed descriptions which involve the eigenvalues and singularities of the meromorphic Floquet matrix function. Existence and size estimates for sequences of spectral gaps are established.

Keywords: Floquet theory, quantum graphs, spectral gaps.

1 Introduction

Among the interesting problems posed by nanoscale technology is the analysis of propagation in periodic networks. Such networks might be used to describe paths for quantum mechanical electron propagation in 'wires' which are macroscopic in length, but have atomic scale width and thickness. These geometries are seen for instance in single wall carbon nanotubes [17]. In addition to electron propagation, there are analogous problems for acoustic or thermal propagation on such networks. Motivated in part by these applications, this work considers spectral problems for differential equations on certain periodic graphs.

Two methods of spectral analysis are available for periodic differential equations. The direct integral analysis typically used for partial differential equations [13, 16] offers broad applicability, but makes sacrifices in detail. The Floquet matrix analysis most common for ordinary differential equations is not as flexible, but often provides more detailed information and sharper results. This work uses the Floquet matrix approach to analyze products of finite graphs $\mathbb{G}$ with the integer graph $\mathbb{Z}$. The vertices of $\mathbb{Z}$ are the integers, and vertices $m, n \in \mathbb{Z}$ are connected by an edge if and only if $n = m \pm 1$. If $V_{\mathbb{G}}$ and $V_{\mathbb{Z}}$ denote the vertex sets of $\mathbb{G}$ and $\mathbb{Z}$ respectively, then the graph product $\mathcal{G} = \mathbb{G} \times \mathbb{Z}$ has vertices (v, n) for $v \in V_{\mathbb{G}}$ and $n \in V_{\mathbb{Z}}$. Vertices (v_1, n_1) and (v_2, n_2) are connected in $\mathcal{G}$ if and only if $n_1 = n_2$ and v_1, v_2 are connected in $\mathbb{G}$, or $v_1 = v_2$ and n_1, n_2 are connected in $\mathbb{Z}$. The edges of $\mathbb{G}$ are assumed to connect distinct vertices.

Our differential operators on the graph $\mathcal{G}$ are actually operators $\mathcal{L} = -D^2 + q$ on the Hilbert space $\oplus_{e \in \mathcal{G}} L^2(e)$. That is, the operators act on functions defined on a set of intervals indexed by the abstract edges of the graph. The edges of $\mathbb{Z}$ will have length 1 and may be identified with the intervals $[m, m+1]$; the resulting topological graph $\mathbb{Z}$ may be identified with the real line, with global coordinate x. The $N(E)$ edges of $\mathbb{G}$ will have lengths r_i, for $i = 1, \dots, N(E)$, and local coordinate t_i, with $0 < t_i < r_i$. Edge lengths for $\mathcal{G}$ are induced in the obvious way, and points on an edge of $\mathcal{G}$ may be described by pairs (v, x) for $v \in V_{\mathbb{G}}$, or (t_i, m) for $m \in V_{\mathbb{Z}}$. The group of integers acts on $\mathcal{G}$ by $n : (v, x) \to (v, x + n)$ and $n : (t_i, m) \to (t_i, m + n)$. An example of a graph $\mathcal{G}$ is illustrated in Figure 1.

The eigenvalue equation

$$(-D^2 + q)y = \lambda y, \quad \lambda \in \mathbb{C}. \tag{1}$$

is basic to this study. The function y is complex valued on each edge, and the potential q is assumed to be real valued, measurable, bounded, and invariant under the action by the group of integers. (The requirement that q be bounded can certainly be relaxed, [7, p. 97], [10, pp. 343–346].)

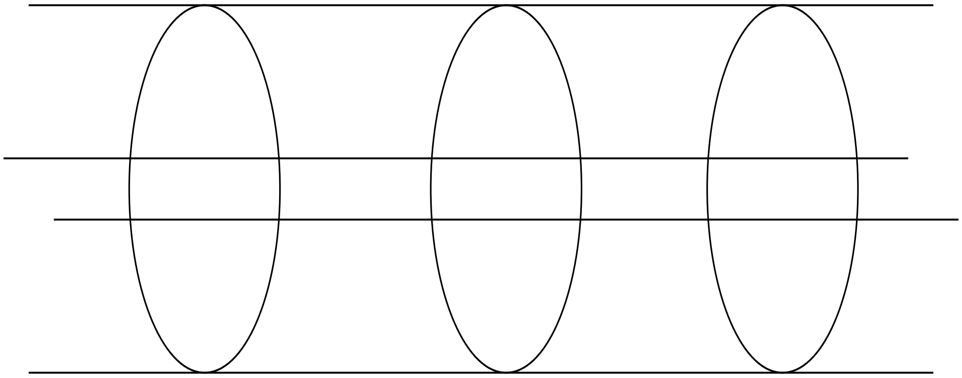

Figure 1

A type of boundary value problem is created by using the structure of $\mathcal{G}$ to define vertex condition constraints on admissible solutions to (1). Denote by y_e the function y restricted to the edge e, and write $e \sim v$ if the vertex v is an endpoint of the edge e. The conditions are

$$\lim_{t \to v} y_{e(1)}(t) = \lim_{t \to v} y_{e(2)}(t), \quad e(1), e(2) \sim v, \tag{2}$$

$$\sum_{e \sim v} \lim_{t \to v} \partial_\nu y_e(t) = 0.$$

The first condition requires continuity of y at the vertices of $\mathcal{G}$. In the second condition $\partial_\nu y_e(t)$ is the derivative in outward pointing local coordinates, so in a fixed set of local coordinates $\partial_\nu y_e(t) = y_e'(t)$ if t is decreasing as t approaches v along e, otherwise $\partial_\nu y_e(t) = -y_e'(t)$. These vertex conditions may be used to define a domain on which $\mathcal{L} = -D^2 + q$ is self adjoint on the Hilbert space $\oplus_{e \in \mathcal{G}} L^2(e)$. Details are provided in [4, 5].

In overview the development unfolds as follows. On the edges of $\mathcal{G}$ where x is not an integer, (1) is a system of ordinary differential equations on intervals $m < x < m+1$. Solutions satisfying (2) are linked by transition matrices associated to $\mathbb{G}$, and satisfy an existence and uniqueness theorem like that for differential equations on $\mathbb{R}$, except for λ in a set Σ_D comprising the Dirichlet eigenvalues from the edges of $\mathbb{G}$. Simple examples show that points in Σ_D may be eigenvalues of $\mathcal{L}$ on $\mathcal{G}$; this feature of quantum graphs is not present in classical Schrödinger equations with periodic coefficients.

The existence and uniqueness result enables us to construct a Floquet matrix type represention for the action of translation by 1 on the space of solutions to (1) satisfying (2) if $\lambda \notin \Sigma_D$. When the potential q is even on the edges of $\mathbb{G}$, the Floquet matrix is symplectic for $\lambda \in \mathbb{R}$ and has a meromorphic continuation for $\lambda \in \mathbb{C}$ with poles in Σ_D. This combination of structural features is quite helpful in establishing the existence of sequences of spectral gaps.

The spectral theoretic consequences of Floquet theory are developed when q is even on the edges of $\mathbb{G}$. The resolvent $R(\lambda) = (\mathcal{L} - \lambda I)^{-1}$ is constructed in two parts, with a particularly simple representation when $R(\lambda)$ acts on functions which vanish on the subgraphs $\mathbb{G} \times m$. As one expects, the spectrum of $\mathcal{L}$ consists of the set Σ_1 where the Floquet matrix has an eigenvalue of absolute value 1, together with a subset of Σ_D. Having connected the spectrum of $\mathcal{L}$ with the multipliers of the Floquet matrix, the existence of spectral gaps is considered. A rich class of examples with an infinite sequence of gaps is constructed under the unexpected hypothesis that $\mathbb{G}$ is not a bipartite graph. These examples exhibit a robust structure which allows us to establish gap size estimates with minimal symmetry assumptions on the potential.

The recent survey [14] may be consulted for an extensive list of references on the history, physical interpretations, and results in partial differential equations related to this work. The applicability of PDE techniques for the spectral analysis of a broad class of periodic difference operators on graphs was noted in [12]. The use of geometric scatterers to open spectral gaps has been previously explored in other contexts. A periodic problem with wide gaps was discussed in [3]. Recent work [18] on decorated graphs does not require periodicity, and also makes use of meromorphic functions in opening spectral gaps. The paper [19], which treats perturbation theory for eigenvalues of infinite multiplicity inside gaps for a different type of graph, provided some of the motivation for this work. The author thanks Peter Kuchment for helpful comments.

2 The Floquet matrix

2.1 Symplectic matrices and the Wronskian

Some basic material on symplectic matrices [2, p. 219], [11, p. 11] will be helpful. Let

$$J = \begin{pmatrix} 0_N & I_N \\ -I_N & 0_N \end{pmatrix}.$$

A real $2N \times 2N$ matrix T is symplectic if

$$T^t J T = J.$$

Extending this definition, a complex $2N \times 2N$ matrix T is J-unitary if

$$T^* J T = J.$$

The characteristic polynomial $p(\xi) = \det(T - \xi I)$ of a symplectic matrix satisfies [2, p. 226]

$$p(\xi) = \xi^{2N} p(1/\xi),$$

or equivalently, the coefficients a_k of $p(\xi)$ satisfy $a_j = a_{2N-j}$. It follows that the eigenvalues of a symplectic matrix are symmetric with respect to the unit circle and the real axis.

For complex vectors W, Z with $2N$ components w_i, z_i we let

$$\langle W, Z \rangle = \sum_{i=1}^{2N} w_i \overline{z_i}.$$

In terms of this form T is J-unitary if and only if

$$\langle JTW, TZ \rangle = \langle JW, Z \rangle, \quad W, Z \in \mathbb{C}^{2N}.$$

For notational convenience define

$$[W, Z] = \langle JW, Z \rangle, \quad W, Z \in \mathbb{C}^{2N}.$$

Suppose that $Q(x)$ is an $N \times N$ matrix valued function defined on an interval with $Q(x) = Q^*(x)$. The conventional Wronski identity has an extension to equations

$$-Y'' + Q(x)Y = \lambda Y. \tag{3}$$

Taking adjoints gives

$$-(Y^*)(x,\overline{\lambda})'' + Y^*(x,\overline{\lambda})Q(x) = \lambda Y^*(x,\overline{\lambda}).$$

If $U(x,\lambda)$ and $V(x,\lambda)$ are $N \times N$ matrix valued functions satisfying (3) then simple algebra leads to

$$V^*(x,\overline{\lambda})U''(x,\lambda) - (V^*)''(x,\overline{\lambda})U(x,\lambda) = 0,$$

so the matrix Wronskian

$$\mathcal{W}(U(x,\lambda), V(x,\lambda)) = V^*(x,\overline{\lambda})U'(x,\lambda) - (V^*)'(x,\overline{\lambda})U(x,\lambda)$$

is a constant. For notational convenience define

$$L^\sharp(\lambda) = L^*(\overline{\lambda})$$

for matrix functions $L(\lambda)$ of $\lambda \in \mathbb{C}$; then

$$\mathcal{W}(U(x,\lambda), V(x,\lambda)) = V^\sharp U' - (V^\sharp)'U.$$

Suppose the columns of $U(x,\lambda)$ and $V(x,\lambda)$ are U_i and V_i. The matrix Wronskian $\mathcal{W}(U,V)$ has entries

$$\mathcal{W}(U,V)_{ij} = \langle \begin{pmatrix} U_j \\ U_j' \end{pmatrix}(\lambda), J\begin{pmatrix} V_i \\ V_i' \end{pmatrix}(\overline{\lambda})\rangle = -[\begin{pmatrix} U_j \\ U_j' \end{pmatrix}(\lambda), \begin{pmatrix} V_i \\ V_i' \end{pmatrix}(\overline{\lambda})].$$

This gives the following result.

Lemma 2.1. *Suppose that $T(\lambda)$ is a $2N \times 2N$ J-unitary matrix for $\lambda \in \mathbb{R}$, and the $N \times N$ matrix functions $\tilde{U}(x,\lambda)$ and $\tilde{V}(x,\lambda)$ satisfy*

$$\begin{pmatrix} \tilde{U}(x_0,\lambda) \\ \tilde{U}'(x_0,\lambda) \end{pmatrix} = T(\lambda)\begin{pmatrix} U(x_0,\lambda) \\ U'(x_0,\lambda) \end{pmatrix}, \quad \begin{pmatrix} \tilde{V}(x_0,\lambda) \\ \tilde{V}'(x_0,\lambda) \end{pmatrix} = T(\lambda)\begin{pmatrix} V(x_0,\lambda) \\ V'(x_0,\lambda) \end{pmatrix}.$$

Then

$$\mathcal{W}(\tilde{U},\tilde{V})(x_0,\lambda) = \mathcal{W}(U,V)(x_0,\lambda).$$

2.2 Unique continuation

The development of Floquet theory for solutions of (1) satisfying (2) begins with a lemma on unique continuation of solutions. Pick some enumeration of the $N(V)$ vertices of $\mathbb{G}$. On the $N(V)$ edges of $\mathcal{G}$ connecting vertices $(v,0)$ and $(v,1)$, where $0<x<1$, equation (1) may be written as

$$-Y'' + \begin{pmatrix} q_1(x) & 0 & \dots & 0 \\ 0 & q_2(x) & \dots & 0 \\ 0 & 0 & \dots & q_{N(V)}(x) \end{pmatrix} Y = \lambda Y, \quad Y = \begin{pmatrix} y_1(x,\lambda) \\ \vdots \\ y_{N(V)}(x,\lambda) \end{pmatrix} \tag{4}$$

and the vector Y of solutions is uniquely determined by its initial data

$$\begin{pmatrix} Y(0^+,\lambda) \\ Y'(0^+,\lambda) \end{pmatrix}. \tag{5}$$

The set of solutions of (1) has a standard basis which may be written as the columns of the (diagonal) $N(V)\times N(V)$ matrix functions $C(x,\lambda)$, $S(x,\lambda)$ which satisfy (1) for $0<x<1$ with the initial conditions

$$C(0^+,\lambda) = I_{N(V)}, \quad S(0^+,\lambda) = 0_{N(V)}, \tag{6}$$

$$C'(0^+,\lambda) = 0_{N(V)}, \quad S'(0^+,\lambda) = I_{N(V)}.$$

Extend these edges to a fundamental domain in $\mathcal{G}$ by taking

$$\begin{aligned} \mathcal{U}_0 &= (v,x), \quad v\in\mathbb{G}, \quad 0<x<1, \\ \mathcal{U}_1 &= (\mathbb{G},1), \end{aligned}$$

and letting $\mathcal{U} = \mathcal{U}_0 \cup \mathcal{U}_1$.

Let $c_e(t,\lambda), s_e(t,\lambda)$ be the basis of solutions to (1) on e satisfying

$$c_e(0,\lambda) = 1, \quad s_e(0,\lambda) = 0, \tag{7}$$

$$c_e'(0,\lambda) = 0, \quad s_e'(0,\lambda) = 1.$$

Recall [15, p.13] that for t in a bounded interval there is a constant K such that

$$|c_e(t,\lambda) - \cos(t\sqrt{\lambda})| \le K/\sqrt{\lambda}, \quad |s_e(t,\lambda) - \sin(t\sqrt{\lambda})/\sqrt{\lambda}| \le K/\lambda, \tag{8}$$

$$|c_e'(t,\lambda) + \sqrt{\lambda}\sin(t\sqrt{\lambda})| \le K, \quad |s_e'(t,\lambda) - \cos(t\sqrt{\lambda})| \le K/\sqrt{\lambda}, \quad \lambda > 0.$$

Let $\Sigma_{D,e}$ denote the set of Dirichlet eigenvalues for (1) on the edge $e \in \mathbb{G}$, that is, the set of $\lambda \in \mathbb{C}$ for which $s_e(r_i,\lambda) = 0$. Then define

$$\Sigma_D = \bigcup_{e \in \mathbb{G}} \Sigma_{D,e}.$$

Notice that in some cases points in Σ_D will be eigenvalues of $\mathcal{L}$ of infinite multiplicity. Suppose that $q = 0$ in (1), and that all edges of $\mathcal{G}$ have length 1. Then we may piece together the functions $\pm\sin(\pi x)$ on a closed path with four edges to build an eigenfunction which vanishes off these four edges.

Lemma 2.2. *For $\lambda \in \mathbb{C} \setminus \Sigma_D$ each solution of* (1) *on $\mathcal{U}_0$ has a unique continuation to a solution on $\mathcal{G}$ which satisfies the vertex conditions* (2)*. Translation by* 1 *on $\mathcal{G}$ acts linearly on the extended solutions. With respect to the standard basis of initial values* (5) *this linear transformation may be written as multiplication on the left by a $2N(V) \times 2N(V)$ matrix valued function $\mathcal{T}(\lambda)$,*

$$\mathcal{T}(\lambda) = \begin{pmatrix} C(1^+,\lambda) & S(1^+,\lambda) \\ C'(1^+,\lambda) & S'(1^+,\lambda) \end{pmatrix} = T_{\mathbb{G}}(\lambda) \begin{pmatrix} C(1^-,\lambda) & S(1^-,\lambda) \\ C'(1^-,\lambda) & S'(1^-,\lambda) \end{pmatrix}.$$

The $2N(V) \times 2N(V)$ matrix function $T_{\mathbb{G}}(\lambda)$ has a meromorphic continuation to the whole plane with poles only in Σ_D.

Proof. Continuation of solutions to the right will be described. Suppose e is an edge in $\mathbb{G}$ with vertices v_1 and v_2, and local coordinate t increasing from 0 at v_1 to r at v_2. If this copy of $\mathbb{G}$ is at $x = m$, and $y(x,\lambda)$ satisfies (1) along the edge (v_i, x) for $m-1 < x < m$, let

$$y(v_i^-,\lambda) = \lim_{x \uparrow m} y(x,\lambda), \quad y'(v_i^-,\lambda) = \lim_{x \uparrow m} y'(x,\lambda).$$

If $\lambda \notin \Sigma_{D,e}$ then

$$z(t,\lambda) = y(v_1^-,\lambda)c_e(t,\lambda) + [y(v_2^-,\lambda) - y(v_1^-,\lambda)c_e(r,\lambda)]\frac{s_e(t,\lambda)}{s_e(r,\lambda)}$$

is the unique solution of (1) on e with $z(0,\lambda) = y(v_1^-,\lambda)$ and $z(r,\lambda) = y(v_2^-,\lambda)$. It follows that

$$z'(0,\lambda) = [y(v_2^-,\lambda) - y(v_1^-,\lambda)c_e(r,\lambda)]\frac{1}{s_e(r,\lambda)}, \tag{9}$$

and by the Wronski identity

$$z'(r,\lambda) = \frac{y(v_2^-,\lambda)s_e'(r,\lambda) - y(v_1^-,\lambda)}{s_e(r,\lambda)}. \tag{10}$$

If $\lambda \notin \Sigma_D$ then this procedure gives us a unique solution z_e on each edge $e \in \mathbb{G}$. These solutions are continued to the edge (v_i, x) for $m < x < m+1$ by using the initial data satisfying (2),

$$y(v^+) = y(v^-), \quad y'(v^+) = y'(v^-) - \sum_{e \sim v} \partial_\nu z_e(v). \tag{11}$$

Writing v_t for the second vertex of the edge e with vertex v, and using (9), (11) may be expressed as

$$y(v^+) = y(v^-), \tag{12}$$

$$y'(v^+) = y'(v^-) + y(v^-) \sum_{e\sim v} \frac{c_e(r_e,\lambda)}{s_e(r_e,\lambda)} - \sum_{e\sim v} \frac{y(v_t^-)}{s_e(r_e,\lambda)}.$$

In this description the solutions $c_e(t,\lambda)$ and $s_e(t,\lambda)$ satisfy their initial conditions at v, and e has length r_e.

Thus the matrix for transition across the graph $\mathbb{G}$ has the form

$$T_{\mathbb{G}}(\lambda) = \begin{pmatrix} I_N & 0_N \\ H(\lambda) & I_N \end{pmatrix}, \quad N = N(V),$$

where $H(\lambda)$ has entries

$$H_{ij} = \left\{ \begin{matrix} \sum_{e\sim v} c_e(r_e,\lambda)/s_e(r_e,\lambda), & i = j, \\ -1/s_e(r_e,\lambda), & e = (v_i, v_j), \\ 0, & \text{otherwise}. \end{matrix} \right\}. \tag{13}$$

It is straightforward to verify the remaining claims.

□

2.3 Structure of $\mathcal{T}(\lambda)$

A description of the important features of the matrix $\mathcal{T}(\lambda)$ begins with a simple lemma.

Lemma 2.3. *The set of* $\lambda \in \mathbb{C}$ *for which* $\mathcal{T}(\lambda)$ *has an eigenvalue* $\xi(\lambda)$ *with* $|\xi(\lambda)| = 1$ *is a subset of the spectrum of* $\mathcal{L}$*, which is contained in a half line* $[b,\infty) \subset \mathbb{R}$.

Proof. We make two preliminary remarks about $-D^2 + q$. First, each set $\Sigma_{D,e}$ is contained in a half line $[b, \infty) \subset \mathbb{R}$. Second, the operator $\mathcal{L}$ on $L^2(\mathcal{G})$ is self adjoint and bounded below [4], so its spectrum is also contained in some $[b, \infty)$.

Next, observe that if $\lambda \neq \Sigma_D$ and $\mathcal{T}(\lambda)$ has an eigenvalue $\xi(\lambda)$ with $|\xi(\lambda)| = 1$, then λ is in the spectrum of $\mathcal{L}$. The argument is essentially the same as for (1) on the line. Start with initial data which is an eigenvector for $\mathcal{T}(\lambda)$ with eigenvalue ξ. The corresponding solution y of (1) extends to all of $\mathbb{G} \times \mathbb{Z}$, and $y(x+1) = \xi y(x)$. Multiply by a suitable sequence of cutoff functions ϕ_n to construct $z_n = \phi_n y$ in the domain of $\mathcal{L}$ such that $\|z_n\| = 1$ and $\|(\mathcal{L} - \lambda)z_n\| \to 0$. ☐

Theorem 2.4. *The* $2N(V) \times 2N(V)$ *matrix function* $\mathcal{T}(\lambda)$ *is real for* $\lambda \in \mathbb{R}\backslash\Sigma_D$ *and has determinant* 1 *for all* $\lambda \in \mathbb{C}\backslash\Sigma_D$. *For* $\lambda \in \mathbb{C}\backslash\mathbb{R}$ *the eigenvalues (multipliers)* $\xi_k(\lambda)$ *of* $\mathcal{T}(\lambda)$ *fall into two groups,* $\{\xi_k(\lambda) \mid |\xi_k(\lambda)| < 1\}$ *and* $\{\xi_k(\lambda) \mid |\xi_k(\lambda)| > 1\}$, *each group having algebraic multiplicity* $N(V)$. *If the potential* q *is even on the edges of* $\mathbb{G}$ *then* $\mathcal{T}(\lambda)$ *is symplectic for* $\lambda \in \mathbb{R} \setminus \Sigma_D$.

Proof. The formulas for $\mathcal{T}(\lambda)$ and $T_{\mathbb{G}}(\lambda)$ in Lemma 2.2 show that $\mathcal{T}(\lambda)$ is real for $\lambda \in \mathbb{R} \setminus \Sigma_D$. For $0 < x < 1$ the matrix solutions $C(x,\lambda)$, $S(x,\lambda)$ of (4) satisfy the matrix Wronski identity

$$(S^t)'(x,\lambda)C(x,\lambda) - S^t(x,\lambda)C'(x,\lambda) = I_{N(V)}, \quad \lambda \in \mathbb{R},$$

implying that

$$\begin{pmatrix} C(1^-,\lambda) & S(1^-,\lambda) \\ C'(1^-,\lambda) & S'(1^-,\lambda) \end{pmatrix}, \quad \lambda \in \mathbb{R}$$

is symplectic. Since this matrix and $T_{\mathbb{G}}(\lambda)$ have determinant 1 for $\lambda \in \mathbb{R}$, the product formula of Lemma 2.2 and meromorphic continuation show $\mathcal{T}(\lambda)$ has determinant 1 for $\lambda \in \mathbb{C} \setminus \Sigma_D$.

Suppose $q(x)$ is even, that is invariant under reflection through the edge midpoint, on each edge e of $\mathbb{G}$. The nonzero off-diagonal entries $H_{ij}(\lambda)$ in (13) are $-1/s_e(r_e,\lambda)$, with the endpoints of e being v_i and v_j, and v_i identified with $t = 0$ in the local coordinate. In terms of the local coordinate t used for H_{ij}, the coordinate used for computation of H_{ji} will be $r - t$. If $s_e(t,\lambda)$ is the solution of (1) with initial data

$$s_e(0,\lambda) = 0, \quad \frac{ds_e}{dt}(0,\lambda) = 1$$

appearing in H_{ij}, then $\widetilde{s_e}(t,\lambda) = s_e(r-t,\lambda)$ is the solution of (1) with initial data

$$\widetilde{s_e}(r,\lambda) = 0, \quad \frac{d\widetilde{s_e}}{d(r-t)}(r,\lambda) = 1$$

appearing in H_{ji}. Since $s_e(r,\lambda) = \widetilde{s_e}(0,\lambda)$, the matrix $H(\lambda)$ is symmetric. It is now easy to check that $T_{\mathbb{G}}(\lambda)$ and $\mathcal{T}(\lambda)$ are symplectic for $\lambda \in \mathbb{R} \setminus \Sigma_D$.

Since the coefficients $a_j(\lambda)$ of the characteristic polynomial of $\mathcal{T}(\lambda)$ are polynomials in the matrix entries, which are meromorphic in λ, it follows that $a_j(\lambda)$ is meromorphic, with all poles in Σ_D. The identities $a_j(\lambda) = a_{2N-j}(\lambda)$, and the identity $p(\xi,\lambda) = \xi^{2N} p(1/\xi,\lambda)$ are thus valid for $\lambda \in \mathbb{C} \setminus \Sigma_D$. For $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the matrix $T(\lambda)$ has no eigenvalues on the unit circle by the previous lemma. It is not hard to show that that if ξ is an eigenvalue for $\mathcal{T}(\lambda)$, then $1/\xi$ is one too, with the same algebraic multiplicity. This finishes the proof in case q is even on each edge of $\mathbb{G}$.

For q real, but not necessarily even on the edges of $\mathbb{G}$, consider the family of self adjoint operators

$$L(s) = -D^2 + sq, \quad 0 \le s \le 1.$$

Pick $\lambda_0 \in \mathbb{C} \setminus \mathbb{R}$. When $s = 0$ the multipliers $\xi_k(\lambda_0)$ split into the two clusters as claimed. The matrices $\mathcal{T}(\lambda_0, s)$ depend analytically on s, and no multiplier can have magnitude 1. Thus [10, pp. 67–68] the algebraic multiplicities of $\{|\xi_k(\lambda)| > 1\}$ and $\{|\xi_k(\lambda)| < 1\}$ are independent of s.

□

3 The resolvent and spectrum of $\mathcal{L}$

This section describes the structure of the resolvent $R(\lambda) = (\mathcal{L} - \lambda I)^{-1}$. The analysis of the resolvent will provide a description of the spectrum of $\mathcal{L}$ in terms of the multipliers of the Floquet matrix $\mathcal{T}(\lambda)$. To obtain a relatively simple description of the resolvent, it is convenient to decompose $L^2(\mathcal{G})$ into two closed orthogonal subspaces,

$$L^2(\mathcal{G}) = H_1 \oplus H_2.$$

The subspace H_1 will consist of the square integrable functions which vanish on the subgraphs $(\mathbb{G}, m)$ for $m \in \mathbb{Z}$, while H_2 will consist of the square integrable functions which vanish on all the edges $m < x < m+1$. The subspace H_2 will be further decomposed

$$H_2 = \oplus H_2^m$$

where H_2^m denotes the functions vanishing on the complement of $(\mathbb{G}, m)$.

Let P_1 denote the orthogonal projection from $L^2(\mathcal{G})$ to H_1. The operator $P_1 R(\lambda) P_1 : H_1 \to H_1$ is known as a generalized resolvent for $-D^2 + q$ corresponding to the self adjoint operator $\mathcal{L}$ on the larger space $L^2(\mathcal{G})$. By viewing $-D^2 + q$ on H_1 as the finite system

$$\begin{pmatrix} -D^2 + q_1(x) & 0 & \dots & 0 \\ 0 & -D^2 + q_2(x) & \dots & 0 \\ 0 & 0 & \dots & -D^2 + q_{N(V)}(x) \end{pmatrix} Y = \lambda Y, \tag{14}$$

on an interval (in this case $(-\infty, \infty)$) it is possible to take advantage of previous work on these generalized resolvents [1, 8]. Because of our explicit knowledge of the extension we will actually consider the operator $R(\lambda) : H_1 \to L^2(\mathcal{G})$, rather than the more traditional generalized resolvent. Similar considerations apply to $R(\lambda) : H_2^m \to L^2(\mathcal{G})$.

Following the next pair of linear algebra results, we will typically assume that q is even on the edges of $\mathbb{G}$.

3.1 Linear algebra

The following consequences of the Jordan normal form will be useful.

Lemma 3.1. *$\mathcal{L}$ has no eigenvalues in the complement of* Σ_D.

Proof. Suppose that $\lambda \in \mathbb{C} \setminus \Sigma_D$ and that ψ is an eigenfunction for $\mathcal{L}$ with eigenvalue λ. By Lemma 2.2 ψ is not identically 0 on $0 < x < 1$, and the continuation of ψ to $m < x < m+1$ may be computed by applying $\mathcal{T}^m(\lambda)$ to the vector ϕ of initial data for ψ at $x = 0^+$. The usual Euclidean norm on ϕ is equivalent to the L^2 norm on solutions of (1) on the interval $0 < x < 1$, so the fact that ψ is square integrable means that

$$\|\mathcal{T}^m \phi\| \to 0, \quad m \to \pm\infty, \quad \|\phi\| \neq 0.$$

We will show that this condition is impossible since $\mathcal{T}(\lambda)$ has no eigenvalues equal to 0.

By applying the similarity transformation putting $\mathcal{T}(\lambda)$ into a Jordan normal form, the problem may be reduced to consideration of a matrix with a single Jordan block

$$\mathcal{J} = \begin{pmatrix} \mu & 1 & \dots & 0 \\ 0 & \vdots & \vdots & 0 \\ 0 & \dots & \mu & 1 \\ 0 & \dots & 0 & \mu \end{pmatrix}.$$

Let $X = (x_1, \dots, x_d, 0, \dots, 0)^t$ be a vector with last nonzero entry x_d. Then

$$\mathcal{J}X = \mu X + (x_2, \dots, x_d, 0, 0, \dots, 0)^t,$$

and the d-th component of $\mathcal{J}^m X$ is $\mu^m x_d$. If $\mu \neq 0$ then it is impossible to have $\mathcal{J}^m X \to 0$ for both $m \to \infty$ and $m \to -\infty$. ☐

Lemma 3.2. *Suppose that $r(\lambda)$ is an $N \times N$ matrix function continuous at λ_0. If all eigenvalues of $r(\lambda_0)$ have magnitude less than 1, then there is a neighborhood B of λ_0 and a positive integer k such that*

$$\|r^k(\lambda)\| < 1, \quad \lambda \in B.$$

Proof. The matrix $r(\lambda_0)$ is similar to a matrix r_1, $r(\lambda_0) = S^{-1} r_1 S$, where $r_1 = \mathcal{D} + \mathcal{N}$ is the sum of the diagonal matrix $\mathcal{D}$, whose entries are the eigenvalues of $r(\lambda_0)$, and a nilpotent matrix $\mathcal{N}$ of order l commuting with $\mathcal{D}$. It follows that

$$r_1^k = (\mathcal{D} + \mathcal{N})^k = \sum_{j=0}^{l-1} \binom{k}{j} \mathcal{D}^{k-j} \mathcal{N}^j.$$

It is elementary to check that r_1^k, and hence $r^k(\lambda_0)$, have limit 0 as $k \to \infty$. The continuity of $r(\lambda)$ at λ_0 then gives the result. ☐

3.2 A Wronskian computation

Let Σ_1 denote the set of $\lambda \in \mathbb{C}$ for which $|\xi_k(\lambda)| = 1$ for some eigenvalue $\xi_k(\lambda)$. A minor extension of Theorem 2.4 shows that if $\lambda \in \mathbb{C} \setminus (\Sigma_1 \cup \Sigma_D)$ the set of solutions of (1) satisfying (2) has an $N(V)$ dimensional subspace $\mathcal{U}$ on which the translation $y(x) \to y(x+1)$ is invariant with all eigenvalues $\xi_k(\lambda)$ satisfying $|\xi_k| < 1$. Define the analogous subspace $\mathcal{V}$ for $|\xi_k| > 1$. Let $U(x, \lambda)$

and $V(x,\lambda)$ be $N(V)\times N(V)$ matrix valued functions whose columns form bases for $\mathcal{U}$ and $\mathcal{V}$ respectively.

Introduce the notation

$$\mathcal{Y}(x,\lambda) = \begin{pmatrix} U & V \\ U' & V' \end{pmatrix},$$

and notice that

$$\begin{pmatrix} (V^\sharp)' & -V^\sharp \\ -(U^\sharp)' & U^\sharp \end{pmatrix} = -J\mathcal{Y}^\sharp J.$$

Lemma 3.3. *Suppose* $\lambda \in \mathbb{C} \setminus (\Sigma_1 \cup \Sigma_D)$. *Then*

$$J\mathcal{Y}^\sharp J\mathcal{Y} = \begin{pmatrix} W(U,V) & 0_{N(V)} \\ 0_{N(V)} & -W(V,U) \end{pmatrix}.$$

In addition, for each λ *the Wronskian* $W(U,V)$ *is a constant invertible* $N(V)\times N(V)$ *matrix for* $x \in \mathbb{R}\setminus\mathbb{Z}$.

Proof. Assume that $\lambda \in \mathbb{C} \setminus (\Sigma_1 \cup \Sigma_D)$. Direct computation gives

$$J\mathcal{Y}^\sharp J\mathcal{Y} = \begin{pmatrix} W(U,V) & W(V,V) \\ -W(U,U) & -W(V,U) \end{pmatrix}.$$

By our earlier observation the Wronskian comprising the $N(V)\times N(V)$ block entries of this matrix are constant on the intervals $m < x < m+1$. Since

$$\begin{pmatrix} U \\ U' \end{pmatrix}((m+1)^+,\lambda) = \mathcal{T}(\lambda)\begin{pmatrix} U \\ U' \end{pmatrix}(m^+,\lambda)$$

and similarly for V, Lemma 2.1 gives

$$W(U,V)((m+1)^+,\lambda) = W(U,V)(m^+,\lambda).$$

The other blocks also have period 1, so the blocks are independent of $x \in \mathbb{R}\setminus\mathbb{Z}$.

The matrix entries of $W(U,U)$ satisfy both

$$W(U,U)_{ij}(m^+,\lambda) = W(U,U)_{ij}(0^+,\lambda)$$

and

$$W(U,U)_{ij}(m^+,\lambda) = -[\mathcal{T}^m(\lambda)\begin{pmatrix} U_j \\ U_j' \end{pmatrix}(0^+,\lambda), \mathcal{T}^m(\overline{\lambda})\begin{pmatrix} U_j \\ U_j' \end{pmatrix}(0^+,\overline{\lambda})].$$

For $\lambda \in \mathbb{C} \setminus (\Sigma_1 \cup \Sigma_D)$ all eigenvalues of $\mathcal{T}(\lambda)$ acting on the span of the columns of

$$\begin{pmatrix} U_j \\ U_j' \end{pmatrix}$$

have absolute value less than 1, so by Lemma 3.2

$$\lim_{m\to\infty} \mathcal{T}^m(\lambda) \begin{pmatrix} U_j \\ U_j' \end{pmatrix} (0,^+, \lambda) = \begin{pmatrix} 0_{N(V)} \\ 0_{N(V)} \end{pmatrix},$$

and thus $W(U,U) = 0_{N(V)}$. The case $W(V,V)$ is similar.

Finally, since the columns of $\mathcal{Y}$ are a basis of solutions to (1) on $0 < x < 1$, the matrix $\mathcal{Y}(x,\lambda)$ is invertible. This means that $J\mathcal{Y}^\sharp J$ is also invertible. Taking the product we see that $W(U,V)$ is invertible. $\square$

3.3 The Resolvent on H_1

For $\lambda \in \mathbb{C} \setminus (\Sigma_1 \cup \Sigma_D)$ define the $N(V) \times N(V)$ matrix function

$$R_1(x_1,x_2,\lambda) = \begin{array}{ll} U(x_1,\lambda)C_1(\lambda)V^*(x_2,\overline{\lambda}), & x_1 \ge x_2, \\ V(x_1,\lambda)C_1^*(\overline{\lambda})U^*(x_2,\overline{\lambda}), & x_1 \le x_2. \end{array} \tag{15}$$

where $C_1(\lambda) = W^{-1}(U,V)$. The function $R_1(x_1,x_2,\lambda)$ may then be used to define an integral operator, initially defined for vector functions on the interval $m < x < m+1$;

$$(R_1(\lambda)f)(x_1) = \int_m^{m+1} R_1(x_1,x_2,\lambda)f(x_2)\,dx_2.$$

Theorem 3.4. *For $f \in \oplus_{N(V)} L^2(m,m+1)$ and $\lambda \in \mathbb{C} \setminus \mathbb{R}$, the integral operator $R_1(\lambda)$ is a representation of the resolvent $(\mathcal{L} - \lambda I)^{-1}$. The function $R_1(\lambda)f$ in $L^2(\mathcal{G})$ extends analytically to $\lambda \in \mathbb{C} \setminus (\Sigma_D \cup \Sigma_1)$.*

Proof. A direct computation shows that if

$$g(x_1) = \int_{\mathbb{R}} R(x_1,x_2,\lambda)f(x_2)\,dx_2,$$

then $(-D^2 + q - \lambda)g = f$ as long as the equations

$$U(x,\lambda)C_1(\lambda)V^*(x,\overline{\lambda}) - V(x,\lambda)C_1^*(\overline{\lambda})U^*(x,\overline{\lambda}) = 0, \tag{16}$$

$$U'(x,\lambda)C_1(\lambda)V^*(x,\overline{\lambda}) - V'(x,\lambda)C_1^*(\overline{\lambda})U^*(x,\overline{\lambda}) = I_{N(V)},$$

are satisfied.

Using Lemma 3.3, these equations are equivalent to

$$J\mathcal{Y}^*(\overline{\lambda})J\mathcal{Y}\begin{pmatrix} C_1(\lambda)V^* \\ -C_1^*(\overline{\lambda})U^* \end{pmatrix} = \begin{pmatrix} V^* \\ -U^* \end{pmatrix},$$

or

$$\begin{pmatrix} W(U,V) & 0_N \\ 0_N & -W(V,U) \end{pmatrix}\begin{pmatrix} C_1(\lambda)V^* \\ -C_1^*(\overline{\lambda})U^* \end{pmatrix} = \begin{pmatrix} V^* \\ -U^* \end{pmatrix},$$

which is satisfied if $C_1(\lambda) = W(U,V)^{-1}$.

Moreover if f has compact support in the interval $(m, m+1)$ then the vertex conditions (2) are satisfied because g is a linear combination of the columns of U for $x > m+1$ and V for $x < m$. Moreover g is square integrable on $\mathcal{G}$ because of the decay of U as $x \to \infty$ and V as $x \to -\infty$ implied by Lemma 3.2.

To establish the analytic continuation we want to show that the columns of $U(x,\lambda)$ and $V(x,\lambda)$ can be chosen as analytic functions with square integrable values on the appropriate 'half graph'. For $\lambda_0 \in \mathbb{C} \setminus (\Sigma_D \cup \Sigma_1)$, pick a basis for the initial data for the functions in $\mathcal{U}$ at λ_0. For λ near λ_0 there is [10, pp. 368–369] a projection onto the generalized eigenspaces with $|\xi_k(\lambda)| < 1$ which is analytic in λ. The extension from analytic initial data to analytic square integrable functions solving (1) with conditions (2) is then completed with the aid of Lemma 3.2. □

Theorem 3.5. *For $\lambda \in \mathbb{C} \setminus (\Sigma_D \cup \Sigma_1)$ the operator $R_1(\lambda)$ is bounded on H_1.*

Proof. Assume that $f \in H_1$, and decompose $f = \sum f_m$, where the projection $f_m = 1_{\{m<x<m+1\}}f$ vanishes unless $m < x < m+1$. We consider the calculation of $g_l(x_1) = R_1(\lambda)f$ for $l < x_1 < l+1$. If $\tilde{f}_m(x_2) = f_m(x_2+m)$, the periodicity of $\mathcal{L}$ gives

$$g_l(x_1) = (R(\lambda)f_m(x_2+m))(x_1) = (R(\lambda)\tilde{f}_m(x_2))(x_1-m), \quad 0 < x_2 < 1.$$

The value of $g(x_1)$ for $x_1 < 0$ is determined by the value for $-1 < x < 0$ and the unique continuation of solutions of (1) satisfying (2). For instance if $l < m$ we see that

$$(R(\lambda)\tilde{f}_m(x_2))(x_1-m) = \int_0^1 V(x_1-m,\lambda)C_1^*(\overline{\lambda})U^*(x_2,\overline{\lambda})\tilde{f}_m(x_2)\,dx_2$$

$$= \int_0^1 V(x_1 - (m-l) - 1), \lambda) C_2^{m-l-1}(\lambda) C_1^*(\overline{\lambda}) U^*(x_2, \overline{\lambda}) \tilde{f}_m(x_2)\, dx_2.$$

The columns of the shifted matrix V are linear combinations of the unshifted version, the transformation for a shift by 1 being given by C_2, which has eigenvalues $\xi_k(\lambda)$ with $|\xi_k(\lambda)| < 1$. Lemma 3.2 shows that we have exponential decay of the iterates. Thus there is a number $0 < \epsilon(\lambda) < 1$ (essentially the value of $|\xi_k|$ closest to 1) such that

$$\int_{-\infty}^{\infty} |g(x_1)|^2 \le \sum_{l=-\infty}^{\infty} \int_l^{l+1} |g_l(x_1)|^2 \le C \sum_l (\sum_m \epsilon^{|l-m|} \|f_m\|)^2.$$

Notice that

$$\sum_m \epsilon^{|l-m|} \|f_m\|$$

is the discrete convolution of the sequences $\{\|f_m\|\}$ and $\epsilon^{|m|}$. By using Fourier series this convolution is a bounded operator on l^2. Thus

$$\sum_l (\sum_m \epsilon^{|l-m|} \|f_m\|)^2 \le C \sum_m \|f_m\|^2,$$

and the integral operator with kernel $R_1(x_1, x_2, \lambda)$ is a bounded operator on H_1 as long as $\lambda \in \mathbb{C} \setminus (\Sigma_D \cup \Sigma_1)$.

□

3.4 The resolvent on H_2^m

We turn next to the structure of the resolvent acting on functions $f \in H_2^m$. Assume at the start that $\lambda \in \mathbb{C} \setminus \mathbb{R}$. Pick an edge $e \in (\mathbb{G}, m)$ and take $f \in L^2(e)$, using local coordinates t for e with $0 < t < r$. Since the resolvent is a right inverse for $\mathcal{L} - \lambda I$ on the interval $0 < t < r_i$ we may write

$$g(t, \lambda) = R(\lambda) f = \alpha c(t, \lambda) + \beta s(t, \lambda) + \int_0^t G(t, \tau) f(\tau)\, d\tau, \quad 0 < t < r, \tag{17}$$

where $c(t, \lambda, q_e)$ and $s(t, \lambda, q_e)$ are the solutions of $-y'' + q_e(t_i) y = \lambda y$ satisfying

$$c(0, \lambda) = 1, \quad s(0, \lambda) = 0,$$

$$c'(0, \lambda) = 0, \quad s'(0, \lambda) = 1,$$

and

$$G(t,\tau,\lambda) = c(t,\lambda)s(\tau,\lambda) - s(t,\lambda)c(\tau,\lambda)$$

is the usual variation of parameters kernel.

Beyond the single edge e the function $g(t,\lambda)$ must extend to a solution of (1) satisfying (2) on $\mathcal{G}$. It must also be square integrable on $\mathcal{G}$. Given choices of local coordinates t_i for the other edges of $\mathbb{G}$, the extended function $g(t,\lambda)$ will have the form

$$g(t,\lambda) = \alpha_i c(t_i,\lambda) + \beta_i s(t_i,\lambda), \quad 0 < t_i < r_i. \tag{18}$$

On the edges with $x > m$ and $x < m$ respectively, the fact that the vertex conditions and square integrability must be satisfied, together with Lemma 3.2, forces g to be a linear combination of the columns U_k and V_k of the previously defined $N(V) \times N(V)$ matrix functions $U(x,\lambda)$ and $V(x,\lambda)$,

$$\sum_k \gamma_k U_k, \quad x > m, \quad \sum_k \delta_k V_k, \quad x < m. \tag{19}$$

The continuity requirement at the vertices of $\mathbb{G}$ gives

$$\sum_k \gamma_k U_k(m^+,\lambda) = \sum_k \delta_k V_k(m^-,\lambda).$$

Let ν be a vertex of $\mathbb{G}$. For edges of $\mathbb{G}$ incident on ν, let I_ν denote the set of edge indices i for which ν has local coordinate 0, and let J_ν denote the set of edge indices i for which ν has local coordinate r_i. At vertices $\nu \in \mathbb{G}$ not belonging to the edge e which contains the support of f, the vertex conditions take the form

$$\sum_k \gamma_k U_k(\nu,\lambda) = \sum_k \delta_k V_k(\nu,\lambda) \tag{20}$$

$$= \alpha_i = \alpha_j c(r_j,\lambda) + \beta_j s(r_j,\lambda), \quad i \in I_\nu, j \in J_\nu,$$

$$\sum_k \gamma_k U_k'(\nu,\lambda) - \sum_k \delta_k V_k'(\nu,\lambda) + \sum_{i\in I_\nu} \beta_i - \sum_{j \in J_\nu} [\alpha_j c'(r_j,\lambda) + \beta_j s'(r_j,\lambda)] = 0.$$

This form also holds at the vertex where the local coordinate on e (which contains the support of f) is 0. At the vertex ν where the local coordinate on e is r the vertex conditions have the modified form

$$\sum_k \gamma_k U_k(\nu,\lambda) = \sum_k \delta_k V_k(\nu,\lambda) = \alpha c(r,\lambda) + \beta s(r,\lambda) \tag{21}$$

$$+\int_0^r G(r,\tau)f(\tau)\ d\tau = \alpha_i = \alpha_j c(r_j,\lambda) + \beta_j s(r_j,\lambda), \quad i \in I_\nu, j \in J_\nu,$$

$$\sum_k \gamma_k U_k'(\nu,\lambda) - \sum_k \delta_k V_k'(\nu,\lambda) + \sum_{i\in I_\nu} \beta_i - \sum_{j \in J_\nu'} [\alpha_j c'(r_j,\lambda) + \beta_j s'(r_j,\lambda)]$$

$$-\alpha c'(r,\lambda) - \beta s'(r,\lambda) = \int_0^r \partial_t G(r,\tau) f(\tau)\ d\tau.$$

Since each edge has two distinct endpoints, these equations have $2N(E)+2N(V)$ unknowns α_i, β_i, γ_k, and δ_k. If a vertex $\nu \in \mathbb{G}$ has degree d, and so degree $d+2$ in $\mathcal{G}$, then the full set of continuity conditions may be written as a set of $d(\nu)+1$ equations. There is one additional equation for the derivatives at ν. We thus have $\Sigma_\nu[d(\nu)+2] = 2N(V)+2N(E)$ equations. Each solution of this linear system provides a solution to the equation $(\mathcal{L}-\lambda I)g = f_e$. Since λ is in the resolvent set there is a unique solution, so our linear system has unique solutions and the coefficient matrix is invertible.

The entries of the coefficient matrix $M(\lambda)$ are either entire functions of λ, or are one of $U_k(\nu,\lambda)$, $V_k(\nu,\lambda)$, $U_k'(\nu,\lambda)$, $V_k'(\nu,\lambda)$. As observed earlier, the vector functions U_k, V_k may be chosen to be analytic for $\lambda \in \mathbb{C} \setminus (\Sigma_D \cup \Sigma_1)$. Consequently the determinant of $M(\lambda)$ can only vanish at a discrete set $\Sigma_2 \subset \mathbb{C} \setminus (\Sigma_D \cup \Sigma_1)$. From here the argument that $R(\lambda) : H_2 \to L^2(\mathcal{G})$ extends to $\mathbb{C} \setminus (\Sigma_D \cup \Sigma_1 \cup \Sigma_2)$ as a bounded linear operator (as well as the analytic continuation argument) is similar to that of Theorem 3.5.

Since $\mathcal{L}$ is self adjoint, the only possible isolated singularities of the resolvent are eigenvalues. By Lemma 3.1 there are no eigenvalues outside the set Σ_D. Putting these arguments together with Theorem 3.5 gives us the next lemma and the expected identification of the spectrum.

Lemma 3.6. *For $f \in H_2^m$ and $\lambda \in \mathbb{C} \setminus \mathbb{R}$, the resolvent $g(\lambda) = (\mathcal{L}-\lambda I)^{-1} f$ may be represented in the form* (17)*,* (18)*,* (19) *with coefficients satisfying* (20) *and* (21)*. The resolvent extends as a bounded operator valued function to $\mathbb{C} \setminus (\Sigma_D \cup \Sigma_1)$.*

Theorem 3.7. *The spectrum Σ of $\mathcal{L}$ satisfies*

$$\Sigma_1 \subset \Sigma \subset (\Sigma_D \cup \Sigma_1).$$

The classical spectral analysis of a self adjoint ordinary differential operator on an interval continues with the development of spectral measures and eigenfunction expansions [7] and [9, p. 1351]. Although these well-known methods are not directly applicable, their generalization to extensions of symmetric ordinary differential operators on an interval to self adjoint operators on a larger Hilbert space may be used. This material is discussed in [1, pp. 121–139], and [8]. For the operators considered here, the abstract extension theory of symmetric operators in larger spaces is enriched by the more or less explicit description of the resolvent based on Floquet matrices.

4 Spectral gaps

The structure of the Floquet matrix for translation by 1 was identified in Lemma 2.2 and made use of the matrix $H(\lambda)$ defined in (13). In light of Theorem 3.7, the structure of $H(\lambda)$ can guarantee the existence of spectral gaps.

Theorem 4.1. *Assume that the edges of* $\mathbb{G}$ *are all of equal length, with the same real even potential. For* λ *near* $\lambda_0 \in \Sigma_D$ *the function* $\mathcal{T}(\lambda)$ *has a Laurent expansion*

$$\mathcal{T}(\lambda) = (\lambda - \lambda_0)^{-1}[\begin{pmatrix} 0_{N(V)} & 0_{N(V)} \\ H_0 C(\lambda_0) & H_0 S(\lambda_0) \end{pmatrix} + (\lambda - \lambda_0) F(\lambda)], \tag{22}$$

with $F(\lambda)$ *analytic. If*

$$\begin{pmatrix} 0_{N(V)} & 0_{N(V)} \\ H_0 C(\lambda_0) & H_0 S(\lambda_0) \end{pmatrix} \tag{23}$$

has $N(V)$ *nonzero eigenvalues, counted with algebraic multiplicity, then* $\mathcal{T}(\lambda)$ *has no multipliers of modulus* 1 *for* λ *sufficiently close to* λ_0*.*

Proof. Since the edges of $\mathbb{G}$ are all of equal length, with the same real even potential, the functions $s(\lambda) = s_e(r, \lambda)$ are all the same. Formula (13) shows that $H(\lambda)$ is meromorphic, with at worst simple poles at the roots of $s(\lambda)$. The Floquet matrix has the form

$$\mathcal{T}(\lambda) = \begin{pmatrix} C(1^-, \lambda) & S(1^-, \lambda) \\ HC(1^-, \lambda) + C'(1^-, \lambda) & HS(1^-, \lambda) + S'(1^-, \lambda) \end{pmatrix}. \tag{24}$$

Suppose that λ_0 is a root of $s(\lambda)$. Then we may expand $\mathcal{T}(\lambda)$ to get (22).

Suppose the $2N(V) \times 2N(V)$ matrix (23) has $N(V)$ nonzero eigenvalues, counted with algebraic multiplicity. Then $\mathcal{T}(\lambda)$ has $N(V)$ multipliers $\xi_k(\lambda)$ (counted with algebraic multiplicity) satisfying

$$\lim_{\lambda \to \lambda_0} |\xi_k(\lambda)| \to \infty.$$

In particular these eigenvalues are not of modulus 1, and since $\mathcal{T}(\lambda)$ is symplectic for $\lambda \in \mathbb{R} \setminus \Sigma_D$, no multipliers of $\mathcal{T}(\lambda)$ have modulus 1 for λ near $\lambda_0 \in \Sigma_D$.

□

For the next results we introduce two matrices containing combinatorial information about $\mathbb{G}$. The $N(V) \times N(V)$ adjacency matrix $A_{\mathbb{G}}$ has entries $a_{ij} = 1$ if vertices v_i and v_j are connected, and 0 otherwise. $\mathcal{D}$ will denote the constant diagonal matrix

$$\mathcal{D} = \mathrm{diag}[deg(v_1), \dots, deg(v_{N(V)})],$$

whose entries are the degrees, or number of incident edges, for the vertices v_i. To see the role of this combinatorial data in the location of spectral gaps some simplifying assumptions are made. Use the notation of (7) for solutions of (1) on $e \in \mathbb{G}$, and let $c(x, \lambda)$ and $s(x, \lambda)$ be the analogous solutions on an edge with $0 < x < 1$ and initial data given at 0^+.

Theorem 4.2. *Suppose that the edges of $\mathbb{G}$ are all of equal length, with the same real even potential q_e, and that the edges with $0 < x < 1$ have the same real potential q_0. Suppose that $\lambda_0 \in \Sigma_D$ and $s(1, \lambda_0) \neq 0$. Then $\mathcal{T}(\lambda)$ has no multipliers of modulus 1 for λ sufficiently close to λ_0 if*

$$\det[c_e(r, \lambda_0)\mathcal{D} - A_{\mathbb{G}}] \neq 0. \tag{25}$$

Condition (25) is satisfied at an infinite sequence of such λ_0 if 2 is not an eigenvalue of $\mathcal{L}_c = I - \mathcal{D}^{-1/2} A_{\mathbb{G}} \mathcal{D}^{-1/2}$.

Proof. For notational convenience the functions $s_e(r, \lambda)$, $s(1, \lambda)$, etc. are written as $s_e(\lambda)$, $s(\lambda)$, etc. With these assumptions the matrix $H(\lambda)$ then has the form

$$H(\lambda) = \frac{1}{s_e(\lambda)}[c_e(\lambda)\mathcal{D} - A_{\mathbb{G}}].$$

The matrices $C(1^-, \lambda), \dots, S'(1^-, \lambda)$ are now scalar, so (24) becomes

$$\mathcal{T}(\lambda) = \begin{pmatrix} 0_N & 0_N \\ c(\lambda)H(\lambda) & s(\lambda)H(\lambda) \end{pmatrix} + \begin{pmatrix} c(\lambda)I_N & s(\lambda)I_N \\ c'(\lambda)I_N & s'(\lambda)I_N \end{pmatrix}$$

$$= \frac{1}{s_e(\lambda)}[M_1(\lambda) + s_e(\lambda)M_2(\lambda)], \quad N = N(V),$$

where

$$M_1(\lambda) = s(\lambda) \begin{pmatrix} 0_N & 0_N \\ \frac{c(\lambda)}{s(\lambda)}[c_e(\lambda)\mathcal{D} - A_{\mathbb{G}}] & [c_e(\lambda)\mathcal{D} - A_{\mathbb{G}}] \end{pmatrix},$$

$$M_2(\lambda) = \begin{pmatrix} c(\lambda)I_N & s(\lambda)I_N \\ c'(\lambda)I_N & s'(\lambda)I_N \end{pmatrix}.$$

Since $s(\lambda_0) \neq 0$ the nonzero eigenvalues of $M_1(\lambda_0)$, counted with algebraic multiplicity, are those of $s(\lambda_0)[c_e(\lambda_0)\mathcal{D} - A_{\mathbb{G}}]$. By assumption there are $N(V)$ nonzero eigenvalues. Since $s_e(\lambda_0) = 0$ the same holds for $M_1(\lambda) + s_e(\lambda)M_2(\lambda)$. By Theorem 4.1 $\mathcal{T}(\lambda)$ has no multipliers of modulus 1 for λ sufficiently close to λ_0.

Note that

$$c_e(\lambda)\mathcal{D} - A_{\mathbb{G}} = \mathcal{D}^{1/2}[c_e(\lambda) - \mathcal{D}^{-1/2}A_{\mathbb{G}}\mathcal{D}^{-1/2}]\mathcal{D}^{1/2}.$$

The estimates (8) give $c_e(\lambda_0) \to \pm 1$ for large $\lambda_0 \in \Sigma_D$. For $c_e(\lambda_0)$ sufficiently close to -1, the matrix $c_e(\lambda_0)\mathcal{D} - A_{\mathbb{G}}$ will be invertible if

$$-I - \mathcal{D}^{-1/2}A_{\mathbb{G}}\mathcal{D}^{-1/2} = \mathcal{L}_c - 2I$$

is invertible, which establishes the last conclusion. □

Notice that $\mathcal{L}_c$ is the combinatorial Laplacian of $\mathbb{G}$ in the sense of Chung [6, p. 3]. The combinatorial Laplacian of a connected graph will have 2 as an eigenvalue if and only if it is bipartite [6, p. 7].

The next theorem shows that the existence of a sequence of spectral gaps guaranteed by Theorem 4.2 is typically a property of the graph $\mathbb{G}$, and not the potential q. The following preparatory lemma considers the stability of matrix eigenvalues under certain types of perturbations.

Lemma 4.3. *Suppose that M is a $2N \times 2N$ matrix*

$$M = A + P = \begin{pmatrix} A_{11} & 0_N \\ 0_N & A_{22} \end{pmatrix} + \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix}$$

whose $N \times N$ blocks satisfy the following conditions:

(i) A_{11} and A_{22} are constant and similar to diagonal matrices.

(ii) The entries of P_{21} are bounded in magnitude by $b > 0$.

(iii) The entries of P_{22} are bounded in magnitude by $\epsilon_1 > 0$.

(iv) The entries of the blocks P_{11} *and* P_{12} *are bounded in magnitude by* $\epsilon_2 > 0$*.*

Then the eigenvalues of M *will converge to those of* A *uniformly as* $\epsilon = \max(\epsilon_1, \epsilon_2, \epsilon_2 b)$ *goes to* 0*.*

Proof. Suppose that $T_1^{-1}A_{11}T_1$ and $T_2^{-1}A_{22}T_2$ are diagonal, and define

$$T = \begin{pmatrix} T_1 & 0_N \\ 0_N & T_2 \end{pmatrix}.$$

Since

$$T^{-1}PT = \begin{pmatrix} T_1^{-1}P_{11}T_1 & T_1^{-1}P_{12}T_2 \\ T_2^{-1}P_{21}T_1 & T_2^{-1}P_{22}T_2 \end{pmatrix},$$

the block estimates are retained up to a constant factor, so there is no loss of generality if A is assumed to be diagonal with eigenvalues $\mu_1, \dots, \mu_{2N}$.

The characteristic polynomial has the standard form

$$p(\mu) = \det(\mu I - M) = \sum_\sigma \operatorname{sgn}(\sigma) \prod_{m=1}^{2N} [\mu I - M]_{m,\sigma(m)}$$

$$= \prod_{m=1}^{2N} (\mu - \mu_m - p_{mm}) + \sum_{k=0}^{2N-1} c_k \mu^k.$$

Suppose that one of the products $\prod_{k=1}^{2N}[\mu I - M]_{k,\sigma(k)}$ contains exactly l factors $b_{i(1)j(1)}, \dots, b_{i(l)j(l)}$ from the block P_{21}. The l diagonal entries with indices $j(1), \dots, j(l)$ are precluded as factors, and since $j(1), \dots, j(l) \le N$ the factors from these rows are $O(\epsilon_2)$. Moreover every coefficient c_k is a sum of products, each product containing at least one offdiagonal factor, so $c_k = O(\epsilon)$ if $0 < \epsilon < 1$.

The proof is completed by recalling that the (suitably ordered) roots of the characteristic polynomial vary continuously with the coefficients. ☐

We will need an arithmetic condition on the length $r > 0$ of the edges of $\mathbb{G}$. Say that r satisfies condition A if the sequence $(2n+1)/r$ contains a subsequence c_k which is uniformly bounded away from the integers. All irrationals r satisfy this condition, but not the rationals $r = 1/m$.

Theorem 4.4. *Assume that* 2 *is not an eigenvalue of* $\mathcal{L}_c = I - \mathcal{D}^{-1/2} A_{\mathbb{G}} \mathcal{D}^{-1/2}$*, and that the edges of* $\mathbb{G}$ *are all of equal length* r*, with even (but possibly distinct) potentials* q_e*. Suppose that* r *satisfies condition A, and that*

$$\lambda_k = c_k^2 \pi^2 = (\frac{2n+1}{r})^2 \pi^2.$$

Pick numbers δ *and* σ *with*

$$0 < \delta < \sigma < 1/2.$$

Then for k *sufficiently large,* $\mathcal{T}(\lambda)$ *has no multipliers of modulus* 1 *for all* λ *satisfying*

$$\lambda_k^{-1/2+\delta} < |\sqrt{\lambda} - \sqrt{\lambda_k}| < \lambda_k^{-1/2+\sigma}, \quad \lambda > 0. \tag{26}$$

Proof. Assume that (26) holds. By the estimates (8) there are bounded functions $K_1(\lambda)$, $K_2(\lambda)$ such that

$$s_e(\lambda) = \frac{\sin(r\sqrt{\lambda})}{\sqrt{\lambda}}[1 + \frac{K_1}{\sqrt{\lambda}\sin(r\sqrt{\lambda})}], \quad c_e(\lambda) = \cos(r\sqrt{\lambda}) + \frac{K_2}{\sqrt{\lambda}}.$$

If k is large enough then by Taylor's Theorem

$$|\sin(r\sqrt{\lambda})| \sim r|\sqrt{\lambda} - \sqrt{\lambda_k}|, \quad \cos(r\sqrt{\lambda}) \sim -1 + O(|\sqrt{\lambda} - \sqrt{\lambda_k}|^2),$$

implying in particular that

$$\frac{r}{2}\lambda^{-1/2+\delta} < |\sin(r\sqrt{\lambda})| < 2r\lambda^{-1/2+\sigma}.$$

For such λ

$$s_e(\lambda) = \frac{\sin(r\sqrt{\lambda})}{\sqrt{\lambda}}[1 + O(\lambda^{-\delta})],$$

$$c_e(\lambda) = -1 + O(\lambda^{\alpha}), \quad \alpha = \max(-1/2, -1 + 2\sigma).$$

Use the abbreviations

$$s_r = \sin(r\sqrt{\lambda})/\sqrt{\lambda}, \quad N_1 = -\mathcal{D} - A_{\mathbb{G}},$$

$$s = \sin(\sqrt{\lambda})/\sqrt{\lambda}, \quad c = \cos(\sqrt{\lambda}).$$

The multipliers of the Floquet matrix are the same as those for

$$\begin{pmatrix} I_N & 0_N \\ 0_N & 1/\sqrt{\lambda} \end{pmatrix} \mathcal{T}(\lambda) \begin{pmatrix} I_N & 0_N \\ 0_N & \sqrt{\lambda} \end{pmatrix} \tag{27}$$

$$= \frac{s}{s_r}\Big[\frac{s_r}{s}\begin{pmatrix} 0_N & 0_N \\ HC(1^-,\lambda)/\sqrt{\lambda} & HS(1^-,\lambda) \end{pmatrix} + \frac{s_r}{s}\begin{pmatrix} C(1^-,\lambda) & \sqrt{\lambda}S(1^-,\lambda) \\ C'(1^-,\lambda)/\sqrt{\lambda} & S'(1^-,\lambda) \end{pmatrix}\Big].$$

The above estimates imply that

$$s_r H(\lambda) = -\mathcal{D} - A_{\mathbb{G}} + o(1), \quad k \to \infty.$$

Condition A insures that $|\sin(\sqrt{\lambda})| \ge \eta > 0$, so that

$$\frac{s_r}{s}\begin{pmatrix} C(1^-,\lambda) & \sqrt{\lambda}S(1^-,\lambda) \\ C'(1^-,\lambda)/\sqrt{\lambda} & S'(1^-,\lambda) \end{pmatrix} = O(\lambda^{-1/2+\sigma}), \quad k \to \infty.$$

The estimates (8) also give

$$C(1^-,\lambda) \simeq \cos(\sqrt{\lambda}) I_N, \quad S(1^-,\lambda) = \frac{\sin(\sqrt{\lambda})}{\sqrt{\lambda}} I_N + O(\lambda^{-1}).$$

Again using $|\sin(\sqrt{\lambda})| \ge \eta > 0$ we find in (27) that

$$\frac{s_r}{s}\begin{pmatrix} 0_N & 0_N \\ HC(1^-,\lambda)/\sqrt{\lambda} & HS(1^-,\lambda) \end{pmatrix}$$

$$= \begin{pmatrix} 0_N & 0_N \\ \frac{\cos(\sqrt{\lambda})}{\sin(\sqrt{\lambda})} N_1[I_N + o(1)] & N_1[I_N + o(1)] \end{pmatrix}.$$

Notice that $-\mathcal{D} - A_{\mathbb{G}}$ is a real symmetric matrix. From Lemma 4.3 the eigenvalues of

$$\frac{s_r}{s}\mathcal{T}(\lambda)$$

approach those of

$$\begin{pmatrix} 0_N & 0_N \\ 0_N & N_1 \end{pmatrix}$$

if

$$\lambda^{-1/2+\sigma}\frac{\cos(\sqrt{\lambda})}{\sin(\sqrt{\lambda})} \to 0,$$

which is insured by condition A. So for λ satisfying (26) and for k sufficiently large, the Floquet matrix $\mathcal{T}(\lambda)$ has N eigenvalues of magnitude bigger than 1. Since $\mathcal{T}(\lambda)$ is symplectic for $\lambda \in \mathbb{R}$, there are no eigenvalues of magnitude 1. ☐

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