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Spectral asymptotics for quantum graphs with equal edge lengths

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Abstract
If q is smooth on the edges of a finite metric graph with all edges of length one, the eigenvalues of the Schrödinger operator $-D^2 + q$ with standard vertex conditions have generalized asymptotic expansions to all orders.

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1. Introduction

In this work, we consider the problem of providing an asymptotic description for the eigenvalues of a Schrödinger operator on a finite metric graph $\mathcal{G}$ with $N_{\mathcal{E}}$ edges. All edges are assumed to have length 1, and the operators have the form $-D^2 + q$ where q is a smooth function on the edges. Eigenfunctions are required to satisfy the standard 'continuity plus Kirchhoff' conditions at interior vertices, and either a Dirichlet condition $y(v) = 0$ or a Neumann condition $y'(v) = 0$ at boundary vertices.

Typically the first such eigenvalue estimate is the 'Weyl estimate'. For $\lambda > 0$ let $\rho(\lambda)$ be the number of eigenvalues less than or equal to λ. As has been noted by previous authors [1–3], one has $\rho(\lambda) \simeq N_{\mathcal{E}}\lambda^{1/2}/\pi$. Hoping to push further, one can consider a Sturm–Liouville problem such as

$$-y'' + py = \lambda y, \qquad y(0) = y(1) = 0, \tag{1.1}$$

with $p \in C^\infty$ as a possible model. For this problem [4] there is a complete asymptotic expansion

$$\lambda_n = n^2\pi^2 + \int_0^1 p(x)\,\mathrm{d}x + \cdots, \tag{1.2}$$

and the eigenvalues λ_n are the roots of the entire function $s(1, \lambda)$, where $s(x, \lambda)$ is the solution of $-y'' + py = \lambda y$ satisfying $y(0, \lambda) = 0$ and $y'(0, \lambda) = 1$.

One encounters several problems in trying to extend such explicit eigenvalue expansions to quantum graphs. The first obstacle already appears in the $q = 0$ case, where previous authors [1–3] have shown that $\lambda \neq n^2\pi^2$ is an eigenvalue if and only if $\cos(\sqrt{\lambda})$ is an eigenvalue of a normalized adjacency matrix. This result guarantees a useful regularity, but it also means that describing eigenvalues is likely to be at least as complicated as root finding for high-degree polynomials.

The operator $-D^2 + q$ on $\mathcal{G}$ may be identified with a boundary value problem for a system of equations on [0, 1]. As in the Sturm–Liouville problem, there is an entire function $\det(\chi_S(\lambda))$ whose zeros are the eigenvalues of $-D^2 + q$. Here $\chi_S(\lambda)$ is a $2N_\mathcal{E} \times 2N_\mathcal{E}$ matrix function. The main work of the paper is to develop an asymptotic expansion for $\chi_S(\lambda)$, with considerable effort expended in the analysis of the first term. In the course of that analysis, we encounter what appears to be a new graph matrix.

The asymptotic expansion of $\chi_S(\lambda)$ and a related matrix function $\chi_F(\lambda)$ has a classical form and depends on $N(J)$ constant coefficients for an order J approximation. The coefficients are obtained by evaluation at 0 and 1 of expressions which are polynomial in the symbols Q, $\frac{\mathrm{d}}{\mathrm{d}x}$ and $\int$. The eigenvalues of $-D^2+q$ can then be approximated by the singular values of the matrix functions which are partial sums of the asymptotic expansions.

With these qualifications about what a generalized asymptotic expansion means, our main result is the following.

Main result. The eigenvalues of the operator $-D^2 + q$ have generalized asymptotic expansions to all orders $J = 1, 2, 3, \ldots$.

As a consequence of our analysis, we are also able to give a reasonably explicit generalization of the two term expansion of (1.2).

We briefly describe the organization of the paper. Section 2 provides a review of previous work and establishes some standard notation. Section 3 introduces the matrix characteristic function $\chi_S(\lambda)$ and the modified characteristic function $\chi_F(\lambda)$. The real work begins in section 4, where a matrix pencil $M_1 + \zeta M_2$ is studied. M_1 and M_2 are $2N_\mathcal{E} \times 2N_\mathcal{E}$ constant matrices which give a description of how to construct the graph from oriented edges. This pencil is central to the error estimates for our expansions. Section 5 develops asymptotic expansions for the characteristic functions, then describes the approximation of eigenvalues by the singular values computed using the expansions. As an application, we show that the addition of the potential q to $-D^2$ causes the eigenvalues λ_n to shift, as $n \to \infty$, by a linear combination of the integrals of q over the edges of $\mathcal{G}$.

The matrix pencil $M_1 + \zeta M_2$, and particularly the matrix $M_1^{-1}M_2$ appear closely related to the bond scattering matrix discussed in [5, 6]. It is likely that a perturbation theory similar to ours could also be developed using these methods. The two approaches appear to have different strengths. The unitary structure of the unperturbed bond scattering matrix is easily verified, while our analysis of the pencil is more indirect. On the other hand our approach, emphasizing an entire characteristic function, seems suitable for inverse spectral problems or algorithms that exploit the sampling theory of entire functions. An explicit translation of these two methods for quantum graphs still seems to be absent, although [7] appears headed in that direction.

2. Some background material

To establish notation and a context for our results, we review some known material about quantum graphs. The propositions in this section are closely related to results in [1, 2]. Additional information may be found in [8, 3] or in the collections [9–11]. For this work a graph $\mathcal{G}$ will be finite, with $N_\mathcal{V}$ vertices and $N_\mathcal{E}$ edges. Every vertex will belong to at least one edge. To avoid minor technical issues, the graph is assumed simple, and all edges have length 1. Multigraphs, graphs with loops, or graphs whose edge lengths are integer multiples of a common value can be easily incorporated by inserting additional vertices.

The edges e_n are initially assumed to be directed and numbered, although this is mainly for notational convenience. Consistent with the edge directions, each edge is identified with the interval [0, 1]. The standard metric and Lebesgue measure on intervals are extended to $\mathcal{G}$. $L^2(\mathcal{G})$ will denote the Hilbert space $\oplus_n L^2(e_n)$ with the inner product

$$\langle f, g\rangle = \int_{\mathcal{G}} f\overline{g} = \sum_{n=1}^{N_\varepsilon} \int_0^1 f_n(x)\overline{g_n(x)}\,\mathrm{d}x, \qquad f = (f_1, f_2, \ldots, fN_\varepsilon).$$

Assume that q is a real-valued function on $\mathcal{G}$, whose restriction to e_n is q_n. The functions q_n will have derivatives $q_n^{(k)}$ of all orders on (0, 1), with each $q_n^{(k)}$ extending continuously to [0, 1]. The function q is not assumed to be continuous on $\mathcal{G}$. A self-adjoint operator $\mathcal{L} = -D^2 + q$, acting componentwise on $f \in L^2(\mathcal{G})$, will have a domain characterized by certain vertex conditions.

At boundary vertices v, which have a single incident edge, either a Dirichlet condition

$$y(v) = 0, \tag{2.1}$$

or a Neumann condition

$$y'(v) = 0, \tag{2.2}$$

will apply. If v is an interior vertex, with degree $\deg(v) > 1$, pick a local indexing $e_1, \ldots, e_{\deg(v)}$ for the edges incident on v. Assume the standard local coordinates, which identify e_n with [0, 1] so that 0 corresponds to v for each edge. At the interior vertex v the standard continuity and derivative (Kirchhoff) conditions apply,

$$y_n(0) = y_{n+1}(0), \qquad n = 1, \ldots, \deg(v) - 1, \qquad \sum_{n=1}^{\deg(v)} y_n'(0) = 0. \tag{2.3}$$

The self-adjoint operator $\mathcal{L}$ will have compact resolvent. Since this operator differs by a finite set of vertex conditions from a collection of $N_{\mathcal{E}}$ decoupled Sturm–Liouville problems, one easily obtains the 'Weyl' estimate.

Proposition 2.1. *Let $\rho(\lambda)$ be the number of eigenvalues of $\mathcal{L}$, counted with multiplicity, that are less than or equal to λ. Then*

$$\rho(\lambda) \simeq \frac{N_{\mathcal{E}}}{\pi}\sqrt{\lambda}.$$

$\mathcal{G}$ also has combinatorial operators acting on the vertex space. Assume that v is a vertex with adjacent vertices $u_1, \ldots, u_{\deg(v)}$. Let $f : \mathcal{V} \to \mathbb{C}$ be a function on the vertex set. Define the normalized adjacency operator by

$$\widehat{A} f(v) = T^{-1}Af(v) = \frac{1}{\deg(v)} \sum_{i=1}^{\deg(v)} f(u_i),$$

where A is the standard adjacency operator, and T is the degree operator $Tf(v) = \deg(v) f(v)$. A simple transformation leads to

$$L_c = T^{1/2}[I - \widehat{A}]T^{-1/2},$$

a much studied operator variously called the Laplacian [12, p 3], the normalized Laplacian, or the analytic Laplacian.

When $q = 0$ the eigenvalues of $\mathcal{L}_0 = -D^2$, which are nonnegative, are closely related to the eigenvalues of $\widehat{A}$. Variations on this theme have been independently developed in the mathematics [1, 2] and physics [13] literature. To summarize these results, suppose $\omega \geqslant 0$, $\lambda = \omega^2$, and $E(\lambda)$ is the eigenspace for $\mathcal{L}_0$ with eigenvalue λ.

The strictly positive eigenvalues occur 'periodically' in ω.

Proposition 2.2. *If* $\omega > 0$,

$$\dim E(\omega^2) = \dim E([\omega + 2n\pi]^2), \qquad n = 1, 2, 3, \ldots.$$

This shows that for $\omega \geqslant 0$ the value of $\rho([\omega + 2\pi]^2) - \rho(\omega^2)$ is a constant, whose value may be obtained from proposition 2.1.

Proposition 2.3. *For* $\omega \geqslant 0$

$$\rho([\omega + 2\pi]^2) - \rho(\omega^2) = 2N_{\mathcal{E}}.$$

Now assume that Neumann conditions apply at boundary vertices.

Proposition 2.4. *If* $\lambda \notin \{n^2\pi^2 \mid n = 0, 1, 2, \ldots\}$, *then* λ *is an eigenvalue of* $\mathcal{L}_0 = -D^2$, *with Neumann conditions at boundary vertices, if and only if* $\cos(\omega) = \cos(\sqrt{\lambda})$ *is an eigenvalue of* $\widehat{A}$, *with the same geometric multiplicity.*

3. Characteristic functions

3.1. Defining the characteristic function

This section will introduce a $2N_{\mathcal{E}} \times 2N_{\mathcal{E}}$ entire matrix function $\chi_S(\lambda)$ whose singular values are the eigenvalues of the quantum graph. To identify graph eigenfunctions with solutions of a system of ordinary differential equations, select a numbering $e_1, \ldots, e_N$ of the $N = N_{\mathcal{E}}$ edges of $\mathcal{G}$, and a set of coordinates identifying each edge with [0, 1]. A function y on $\mathcal{G}$ may then be written as a vector function

$$Y(x) = (y_1(x), \ldots, y_N(x))^T, \qquad 0 \leqslant x \leqslant 1.$$

In this representation, an eigenfunction of the graph operator $-D^2 + q$ will be a solution of the diagonal system

$$-Y'' + Q(x)Y = \lambda Y, \qquad Q(x) = \text{diag}[q_1(x), \ldots, q_N(x)]. \tag{3.1}$$

To satisfy the vertex conditions (2.1), (2.2) or (2.3), such an eigenfunction of the self-adjoint operator $\mathcal{L}$ will satisfy a typically nondiagonal set of $2N$ independent linear boundary conditions, which have the form

$$\begin{gathered}\sum b^1_{mn} y_n(0) + \sum b^2_{mn} y'_n(0) + \sum b^3_{mn} y_n(1) + \sum b^4_{mn} y'_n(1) = 0,\\ m = 1, \ldots 2N, \qquad n = 1, \ldots, N,\end{gathered} \tag{3.2}$$

with coefficients $b^l_{mn} \in \{0, \pm 1\}$. If $B_l = \left(b^l_{mn}\right)$, then the $2N \times 4N$ boundary matrix is

$$B = (B_1, B_2, B_3, B_4). \tag{3.3}$$

A basis of solutions for (3.1) may be identified with a pair of $N \times N$ matrix functions $(Y_1(x, \lambda), Y_2(x, \lambda))$ whose columns are linearly independent solutions. Let I_N denote the

$N \times N$ identity matrix. The standard basis for the diagonal system is $(C(x,\lambda), S(x,\lambda))$, where

$$C(x,\lambda) = \mathrm{diag}[c(x,\lambda,q_1),\ldots,c(x,\lambda,q_N)],$$
$$S(x,\lambda) = \mathrm{diag}[s(x,\lambda,q_1),\ldots,s(x,\lambda,q_N)],$$

which satisfies the initial condition

$$\begin{pmatrix} C(0,\lambda) & S(0,\lambda) \\ C'(0,\lambda) & S'(0,\lambda) \end{pmatrix} = I_{2N}.$$

Lemma 3.1. *Suppose that $(Y_1(x,\lambda), Y_2(x,\lambda))$ is a basis for (3.1). The number $\lambda \in \mathbb{C}$ is an eigenvalue of $-D^2+q$ on $\mathcal{G}$ with geometric multiplicity m_g if and only if the $2N \times 2N$ matrix*

$$\chi(\lambda) = (B_1 \quad B_2 \quad B_3 \quad B_4)\begin{pmatrix} Y_1(0,\lambda) & Y_2(0,\lambda) \\ Y_1'(0,\lambda) & Y_2'(0,\lambda) \\ Y_1(1,\lambda) & Y_2(1,\lambda) \\ Y_1'(1,\lambda) & Y_2'(1,\lambda) \end{pmatrix} \tag{3.4}$$

has a null space of dimension m_g.

Proof. First, suppose $\lambda \in \mathbb{C}$ is an eigenvalue of $-D^2+q$ on $\mathcal{G}$ with geometric multiplicity m_g. Each eigenfunction $Y(x,\lambda)$ is a linear combination of the basis elements of the solutions of (3.1), and there are m_g independent $2N \times 1$ matrices α_i such that

$$Z_i = (Y_1(x,\lambda) \quad Y_2(x,\lambda))\alpha_i$$

gives a basis for the eigenspace. The boundary values of Z_i are

$$\begin{pmatrix} Z_i(0,\lambda) \\ Z_i'(0,\lambda) \\ Z_i(1,\lambda) \\ Z_i'(1,\lambda) \end{pmatrix} = \begin{pmatrix} Y_1(0,\lambda) & Y_2(0,\lambda) \\ Y_1'(0,\lambda) & Y_2'(0,\lambda) \\ Y_1(1,\lambda) & Y_2(1,\lambda) \\ Y_1'(1,\lambda) & Y_2'(1,\lambda) \end{pmatrix}\alpha_i.$$

Since Z_i satisfies the boundary conditions, we have

$$(B_1 \quad B_2 \quad B_3 \quad B_4)\begin{pmatrix} Y_1(0,\lambda) & Y_2(0,\lambda) \\ Y_1'(0,\lambda) & Y_2'(0,\lambda) \\ Y_1(1,\lambda) & Y_2(1,\lambda) \\ Y_1'(1,\lambda) & Y_2'(1,\lambda) \end{pmatrix}\alpha_i = 0,$$

and each vector α_i is a null vector for the $2N \times 2N$ matrix $\chi(\lambda)$.

Conversely, if $\chi(\lambda)$ has a null space of dimension m_g, then we have m_g-independent null vectors α_i, and the independent vectors Z_i defined as above will satisfy the boundary conditions. $\square$

A specific choice of basis may simplify the analysis of $\chi(\lambda)$. Starting with the standard basis for (3.1), define the matrix characteristic function

$$\begin{aligned} \chi_S(\lambda) &= (B_1 \quad B_2 \quad B_3 \quad B_4)\begin{pmatrix} C(0,\lambda) & S(0,\lambda) \\ C'(0,\lambda) & S'(0,\lambda) \\ C(1,\lambda) & S(1,\lambda) \\ C'(1,\lambda) & S'(1,\lambda) \end{pmatrix} \\ &= (B_1 \quad B_2) + (B_3 \quad B_4)\begin{pmatrix} C(1,\lambda) & S(1,\lambda) \\ C'(1,\lambda) & S'(1,\lambda) \end{pmatrix}. \end{aligned} \tag{3.5}$$

The previous lemma and the well-known analyticity of the functions $c(x, \lambda, q_n)$ and $s(x, \lambda, q_n)$ from the standard basis give the next lemma.

Lemma 3.2. *The number $\lambda \in \mathbb{C}$ is an eigenvalue of $-D^2 + q$ on $\mathcal{G}$ if and only if the $2N \times 2N$ entire matrix function $\chi_S(\lambda)$ has determinant 0.*

3.2. A modified characteristic function

Extend the definition $\omega = \sqrt{\lambda}$ to complex $\lambda \notin (-\infty, 0]$. Another convenient basis is

$$(E_+(x,\lambda), E_-(x,\lambda)) = (C(x,\lambda), S(x,\lambda)) \begin{pmatrix} I_N & I_N \\ \mathrm{i}\omega I_N & -\mathrm{i}\omega I_N \end{pmatrix}, \tag{3.6}$$

which has initial values

$$\begin{pmatrix} E_+(0,\lambda) & E_-(0,\lambda) \\ E_+'(0,\lambda) & E_-'(0,\lambda) \end{pmatrix} = \begin{pmatrix} I_N & I_N \\ \mathrm{i}\omega I_N & -\mathrm{i}\omega I_N \end{pmatrix}.$$

If Q is the zero function, then

$$(E_+(x,\lambda), E_-(x,\lambda)) = (\exp(\mathrm{i}\omega x) I_N, \exp(-\mathrm{i}\omega x) I_N).$$

Using (3.6), the basis (E_+, E_-) is associated with a modified characteristic function $\chi_E(\lambda)$, defined by

$$\chi_S(\lambda) = \frac{1}{2}\chi_E(\lambda) \begin{pmatrix} I_N & -\mathrm{i}\omega^{-1} I_N \\ I_N & \mathrm{i}\omega^{-1} I_N \end{pmatrix}, \tag{3.7}$$

where

$$\chi_E(\lambda) = (B_1 \quad B_2 \quad B_3 \quad B_4) \begin{pmatrix} E_+(0,\lambda) & E_-(0,\lambda) \\ E_+'(0,\lambda) & E_-'(0,\lambda) \\ E_+(1,\lambda) & E_-(1,\lambda) \\ E_+'(1,\lambda) & E_-'(1,\lambda) \end{pmatrix}$$

$$= (B_1 \quad B_2) \begin{pmatrix} I_N & I_N \\ \mathrm{i}\omega I_N & -\mathrm{i}\omega I_N \end{pmatrix} + (B_3 \quad B_4) \begin{pmatrix} E_+(1,\lambda) & E_-(1,\lambda) \\ E_+'(1,\lambda) & E_-'(1,\lambda) \end{pmatrix}. \tag{3.8}$$

The form of the vertex conditions now plays an important role. Introducing additional notation, let

$$\zeta = \exp(\mathrm{i}\omega),$$

and let Ω be the $2N \times 2N$ diagonal matrix with kth diagonal entry $\mathrm{i}\omega$ if the kth vertex condition has derivative evaluations, and 1 otherwise. The factorization (3.7) will now be extended.

Lemma 3.3. *The characteristic function $\chi_S(\lambda)$ may be factored as*

$$\chi_S(\lambda) = \frac{1}{2}\Omega\chi_F(\lambda) \begin{pmatrix} I_N & 0_N \\ 0_N & \zeta^{-1} I_N \end{pmatrix} \begin{pmatrix} I_N & -\mathrm{i}\omega^{-1} I_N \\ I_N & \mathrm{i}\omega^{-1} I_N \end{pmatrix}, \qquad \lambda \notin (-\infty, 0], \tag{3.9}$$

with

$$\chi_F(\lambda) = (B_1 \ B_2) \begin{pmatrix} I_N & \zeta I_N \\ I_N & -\zeta I_N \end{pmatrix} + (B_3 \ B_4) \begin{pmatrix} E_+(1,\lambda) & E_-(1,\lambda)\zeta \\ (\mathrm{i}\omega)^{-1} E_+'(1,\lambda) & (\mathrm{i}\omega)^{-1} E_-'(1,\lambda)\zeta \end{pmatrix}. \tag{3.10}$$

Proof. The boundary conditions (3.2) coming from the graph involve either function evaluations or derivative evaluations, but not both. This leads to the identity

$$\Omega^{-1}(B_1 \quad B_2) = (B_1 \quad B_2) \begin{pmatrix} I_N & 0_N \\ 0_N & -\mathrm{i}\omega^{-1} I_N \end{pmatrix}$$

since both products leave fixed the entries of B_1, which express function evaluations, and multiply all nonzero entries of B_2 by $-\mathrm{i}\omega^{-1}$. The same reasoning also gives

$$\Omega^{-1}(B_3 \quad B_4) = (B_3 \quad B_4)\begin{pmatrix} I_N & 0_N \\ 0_N & -\mathrm{i}\omega^{-1}I_N \end{pmatrix}.$$

The desired factorization follows by applying these identities to

$$\chi_E(\lambda) = \Omega\Omega^{-1}(B_1 \quad B_2)\begin{pmatrix} I_N & I_N \\ \mathrm{i}\omega I_N & -\mathrm{i}\omega I_N \end{pmatrix}\begin{pmatrix} I_N & 0_N \\ 0_N & \zeta I_N \end{pmatrix}\begin{pmatrix} I_N & 0_N \\ 0_N & \zeta^{-1}I_N \end{pmatrix}$$
$$+ \Omega\Omega^{-1}(B_3 \quad B_4)\begin{pmatrix} E_+(1,\lambda) & E_-(1,\lambda) \\ E_+'(1,\lambda) & E_-'(1,\lambda) \end{pmatrix}\begin{pmatrix} I_N & 0_N \\ 0_N & \zeta I_N \end{pmatrix}\begin{pmatrix} I_N & 0_N \\ 0_N & \zeta^{-1}I_N \end{pmatrix}. \qquad \square$$

4. Characteristic function $\chi_0(\lambda)$ for $-D^2$

When $Q = 0$ the modified characteristic function $\chi_F(\lambda)$ has the elementary form of a linear pencil $M_1 + \zeta M_2$, in $\zeta = \mathrm{e}^{\mathrm{i}\omega}$, where the constant $2N_\mathcal{E} \times 2N_\mathcal{E}$ matrices are

$$M_1 = (B_1 + B_2 \quad B_3 - B_4), \qquad M_2 = (B_3 + B_4 \quad B_1 - B_2). \tag{4.1}$$

The characteristic function $\chi_S(\lambda)$ in the $Q = 0$ case will be denoted by $\chi_0(\lambda)$. When notationally convenient we take $N = N_\mathcal{E}$. The main features of $M_1 + \zeta M_2$ and

$$\chi_0(\lambda) = (B_1 \quad B_2) + (B_3 \quad B_4)\begin{pmatrix} \cos(\sqrt{\lambda})I_N & \dfrac{\sin(\sqrt{\lambda})}{\sqrt{\lambda}}I_N \\ -\sqrt{\lambda}\sin(\sqrt{\lambda})I_N & \cos(\sqrt{\lambda})I_N \end{pmatrix} \tag{4.2}$$

are described in the next theorem.

Theorem 4.1. *The eigenvalues of $-D^2$ for a graph $\mathcal{G}$ with $N_\mathcal{E}$ edges and standard vertex conditions are the roots of* $\det \chi_0(\lambda)$*, where $\chi_0(\lambda)$ is an entire $2N_\mathcal{E} \times 2N_\mathcal{E}$ matrix function. The geometric multiplicity of the eigenvalue at λ is the dimension of the null space of $\chi_0(\lambda)$. With $\lambda \in \mathbb{C} \setminus (-\infty, 0]$, $\omega = \sqrt{\lambda}$ and $\zeta = \exp(\mathrm{i}\omega)$, the matrix function $\chi_0(\lambda)$ has a factorization*

$$\chi_0(\lambda) = \frac{1}{2}\Omega[M_1 + \zeta M_2]\begin{pmatrix} I_N & 0_N \\ 0_N & \zeta^{-1}I_N \end{pmatrix}\begin{pmatrix} I_N & -\mathrm{i}\omega^{-1}I_N \\ I_N & \mathrm{i}\omega^{-1}I_N \end{pmatrix}, \tag{4.3}$$

where Ω is a $2N_\mathcal{E} \times 2N_\mathcal{E}$ diagonal matrix, with diagonal entries either $\mathrm{i}\omega$ or 1, and M_1 and M_2 are $2N_\mathcal{E} \times 2N_\mathcal{E}$ constant matrices. Except for $M_1 + \zeta M_2$, the matrices appearing in this factorization are invertible, so for $\Re(\omega) > 0$ the number ω^2 is an eigenvalue of $-D^2$ if and only if $\det(M_1 + \zeta M_2) = 0$.

The matrices M_1 and M_2 are invertible, so $\det(M_1 + \zeta M_2) = 0$ *if and only if $-\zeta$ is an eigenvalue of $M_2^{-1}M_1$. Counted with geometric multiplicity, the $2N_\mathcal{E} \times 2N_\mathcal{E}$ matrix $M_2^{-1}M_1$ has $2N_\mathcal{E}$ eigenvalues $-\zeta_1, \ldots, -\zeta_{2N}$, all satisfying $|\zeta_k| = 1$. Suppose* $\det \chi_0(\lambda_1) = 0$ *and $\lambda_1 \neq 0$. Then $\chi_0^{-1}(\lambda)$ has a simple pole at $\lambda = \lambda_1$.*

The claims in the first paragraph of theorem 4.1 have already been established in lemma 3.1, lemma 3.2 and in the development of (3.8) and (3.10). The rest of the proof will be presented in the next pair of lemmas.

Consider the matrix M_1 in a special case. Assume that the vertex v has degree $m \geqslant 2$, that the first m vertex conditions come from v, and that all edges incident on v are oriented so that v is identified with $x = 0$. Then the first $m \times m$ block of M_1 can be assumed to have the form

$$D = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 \\ 0 & 1 & -1 & \dots & 0 \\ 0 & 0 & \vdots & \dots & 0 \\ 0 & 0 & \dots & 1 & -1 \\ 1 & 1 & 1 & \dots & 1 \end{pmatrix}.$$

The matrix D is invertible and provides a model for the next result.

Lemma 4.2. *The matrices M_1 and M_2 are invertible.*

Proof. The proofs are similar for M_1 and M_2, so only the first case is treated. The argument is by contradiction. If M_1 is not invertible there is a nonzero vector $X = (x_1, \dots, x_{2N})^T$ with $M_1 X = 0$. Suppose in particular that $x_k \neq 0$. The cases $1 \leqslant k \leqslant N$ and $N+1 \leqslant k \leqslant 2N$ are similar. Suppose that $1 \leqslant k \leqslant N$, and that v is the vertex corresponding to 0 for the kth edge.

If v has only one incident edge, then either vertex condition (2.1) or (2.2) applies. If this vertex condition is represented by row j of M_1, then the jth component equation for $M_1 X = 0$ is $x_k = 0$, contradicting the assumption that $x_k \neq 0$.

Suppose $\deg(v) = m \geqslant 2$, so vertex conditions (2.3) hold for v. After a reordering of the vertex conditions for all vertices, the vertex conditions for v may be assumed to be the first m conditions, determining the first m rows of M_1. Let $j(1) < \cdots < j(m)$ be the column indices (which include k) with nonvanishing entries in the first m rows of M_1. After applying additional elementary row operations on the first m rows of M_1, which gives equivalent vertex conditions and does not affect the invertibility of M_1, the first m equations of $M_1 X = 0$ may be assumed to have the form

$$x_{j(i)} - x_{j(i+1)} = 0, \qquad i = 1, \dots, m-1, \qquad \sum_{i=1}^{m} x_{j(i)} = 0.$$

Since the values $x_{j(i)}$ are equal, the last equation gives $m x_k = 0$, a contradiction. □

Finding the values of ζ for which $M_1 + \zeta M_2$ has determinant 0 is the same as finding the values of ζ for which

$$\det\left(M_2\left[M_2^{-1} M_1 - \zeta I_N\right]\right) = 0,$$

which is the same as saying ζ should be one of the eigenvalues of the constant matrix $M_2^{-1} M_1$.

The next lemma completes the proof of theorem 4.1.

Lemma 4.3. *Counted with geometric multiplicity, the $2N_{\mathcal{E}} \times 2N_{\mathcal{E}}$ matrix $M_2^{-1} M_1$ has $2N_{\mathcal{E}}$ eigenvalues $\zeta_1, \dots, \zeta_{2N}$, all satisfying $|\zeta_k| = 1$.*

Suppose $\lambda_1 \neq 0$ is an eigenvalue of $-D^2$. Then $\chi_0^{-1}(\lambda)$ has a simple pole at $\lambda = \lambda_1$, and $(M_1 + \exp(\mathrm{i}\omega) M_2)^{-1}$ has a simple pole at $\sqrt{\lambda_1}$.

Proof. The eigenvalues of $-D^2$ are real and nonnegative. Pick a real interval of the form $\mathcal{I} = (\omega_0, \omega_0 + 2\pi)$ with $\omega_0 > 0$ and $\chi_0(\omega_0^2)$ nonsingular. For $k = 1, 2, \dots,$ let $\lambda_k = \omega_k^2$ be the eigenvalues of $-D^2$ for $\omega \in \mathcal{I}$.

First, proposition 2.3 shows that the sum of the geometric multiplicities of the eigenvalues ω_k^2 is $2N_{\mathcal{E}}$. By lemma 3.1 this is the same as the sum of the geometric multiplicities of 0 as an eigenvalue of $\chi_0(\omega_k^2)$, which is the same as the sum of the geometric multiplicities of the $2N_{\mathcal{E}}$ eigenvalues of $M_2^{-1} M_1$ at $\zeta_k = \exp(\mathrm{i}\omega_k)$. Since the sum of the algebraic multiplicities of the eigenvalues of $M_2^{-1} M_1$ is also $2N_{\mathcal{E}}$, all of the eigenvalues are accounted for.

Suppose $\lambda_1 \neq 0$ and $\det \chi_0(\lambda_1) = 0$. Rewrite the factorization of $\chi_0(\lambda)$ as

$$\chi_0(\lambda) = \frac{1}{2}\Omega M_2\left[M_2^{-1}M_1 + \zeta I\right]\begin{pmatrix} I_N & 0_N \\ 0_N & \zeta^{-1}I_N \end{pmatrix}\begin{pmatrix} I_N & -\mathrm{i}\omega^{-1}I_N \\ I_N & \mathrm{i}\omega^{-1}I_N \end{pmatrix}.$$

The factors other than $M_2^{-1}M_1 + \zeta I$ have inverses which are analytic in a neighborhood of λ_1. Since the sum of the geometric multiplicities of the eigenvalues of $M_2^{-1}M_1$ is $2N_{\mathcal{E}}$, the matrix $M_2^{-1}M_1$ is diagonalizable, and $\left(M_2^{-1}M_1 + \zeta I\right)^{-1}$ is similar to

$$\mathrm{diag}[(\zeta_1 + \zeta)^{-1}, \ldots, (\zeta_{2N} + \zeta)^{-1}].$$

The functions

$$f_k(\lambda) = \zeta_k + \zeta = \zeta_k + \exp(\mathrm{i}\sqrt{\lambda})$$

have derivative

$$f_k'(\lambda) = \frac{\mathrm{i}}{2\sqrt{\lambda}}\exp(\mathrm{i}\sqrt{\lambda}).$$

Since the derivatives do not vanish, if f_k has a zero at λ_1, it is a simple zero, so $\chi_0^{-1}(\lambda)$ has a simple pole at λ_1. Essentially the same argument works for $(M_1 + \exp(\mathrm{i}\omega)M_2)^{-1}$. □

5. Asymptotic expansions

This section begins with a review of asymptotic developments for solutions of the scalar equation

$$-y'' + q(x)y = \lambda y, \tag{5.1}$$

and the analogous diagonal matrix equation (3.1).

5.1. Characteristic function asymptotics

Suppose the functions $c(x, \lambda)$ and $s(x, \lambda)$ satisfy (5.1) subject to the initial conditions

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

When $q(x)$ is sufficiently differentiable, elaborate expansions for these functions may be computed. Expansions to all orders for smooth functions q are described in [4, 14]. To indicate the nature of the expansion, if $q \in H^2_{\mathbb{C}}$ and

$$[q] = \int_0^1 q(x)\,\mathrm{d}x,$$

then [15, p 16]

$$c(1, \lambda) = \cos(\sqrt{\lambda}) + [q]\frac{\sin(\sqrt{\lambda})}{2\sqrt{\lambda}} + \left(q(1) - q(0) - \frac{1}{2}[q]^2\right)\frac{\cos(\sqrt{\lambda})}{4\lambda} + O(|\lambda|^{-3/2}\exp(|\Im\sqrt{\lambda}|)),$$

$$c'(1, \lambda) = -\sqrt{\lambda}\sin(\sqrt{\lambda}) + [q]\frac{\cos(\sqrt{\lambda})}{2} + q(1)\frac{\sin(\sqrt{\lambda})}{2\sqrt{\lambda}} - \left(q(1) - q(0) - \frac{1}{2}[q]^2\right)\frac{\sin(\sqrt{\lambda})}{4\sqrt{\lambda}} + O(|\lambda|^{-1}\exp(|\Im\sqrt{\lambda}|)),$$

$$s(1,\lambda) = \frac{\sin(\sqrt{\lambda})}{\sqrt{\lambda}} - [q]\frac{\cos(\sqrt{\lambda})}{2\lambda}$$
$$+\left(q(1)+q(0)-\frac{1}{2}[q]^2\right)\lambda^{-3/2}\frac{\sin(\sqrt{\lambda})}{4} + O(|\lambda|^{-2}\exp(|\Im\sqrt{\lambda}|)),$$
$$s'(1,\lambda) = \cos(\sqrt{\lambda}) + [q]\lambda^{-1/2}\frac{\sin(\sqrt{\lambda})}{2} - q(1)\frac{\cos(\sqrt{\lambda})}{2\lambda}$$
$$+\left(q(1)+q(0)-\frac{1}{2}[q]^2\right)\lambda^{-1}\frac{\cos(\sqrt{\lambda})}{4} + O(|\lambda|^{-3/2}\exp(|\Im\sqrt{\lambda}|)).$$

These expansions extend to the basis of (3.6), since

$$E_\pm(x,\lambda) = C(x,\lambda) \pm \mathrm{i}\sqrt{\lambda}S(x,\lambda).$$

When $x = 1$ the expansions take the form

$$(E_+(1,\lambda) \quad E_-(1,\lambda)) = (E_{J,+}(\omega) \quad E_{J,-}(\omega)) + R_J^0,$$
$$(E_+'(1,\lambda) \quad E_-'(1,\lambda)) = \mathrm{i}\omega\big[(E_{J,+}'(\omega) \quad E_{J,-}'(\omega)) + R_J^1\big],$$

with

$$\|R_J^0(\omega)\| = O(\omega^{-J}), \qquad \|R_J^1(\omega)\| = O(\omega^{-J}).$$

In these expansions,

$$\begin{aligned}(E_{J,+}(\omega) \quad E_{J,-}(\omega)) &= \sum_{m=0}^{J-1}(\mathrm{i}\omega)^{-m}(\exp(\mathrm{i}\omega)I_N \quad \exp(-\mathrm{i}\omega)I_N)\mathcal{A}_m \\ (E_{J,+}'(\omega) \quad E_{J,-}'(\omega)) &= \sum_{m=0}^{J-1}(\mathrm{i}\omega)^{-m}(\exp(\mathrm{i}\omega)I_N \quad \exp(-\mathrm{i}\omega)I_N)\mathcal{B}_m,\end{aligned} \tag{5.2}$$

with $\mathcal{A}_m$ and $\mathcal{B}_m$ being $2N \times 2N$ matrices with complex entries.

As in (3.1), let $Q = \mathrm{diag}[q_1,\ldots,q_N]$. The coefficients for $m = 0, 1, 2$ are

$$\begin{aligned}&\mathcal{A}_0 = \begin{pmatrix} I_N & 0_N \\ 0_N & I_N\end{pmatrix}, \qquad \mathcal{A}_1 = \frac{1}{2}\begin{pmatrix}[Q] & 0_N \\ 0_N & -[Q]\end{pmatrix}, \\ &\mathcal{A}_2 = \frac{1}{8}\begin{pmatrix}[Q]^2 - 2Q(1) & 2Q(0) \\ 2Q(0) & [Q]^2 - 2Q(1)\end{pmatrix}. \\ &\mathcal{B}_0 = \begin{pmatrix} I_N & 0_N \\ 0_N & -I_N\end{pmatrix}, \qquad \mathcal{B}_1 = \frac{1}{2}\begin{pmatrix}[Q] & 0_N \\ 0_N & [Q]\end{pmatrix}, \\ &\mathcal{B}_2 = \frac{1}{8}\begin{pmatrix}[Q]^2 + 2Q(1) & -2Q(0) \\ 2Q(0) & -[Q]^2 - 2Q(1)\end{pmatrix}.\end{aligned} \tag{5.3}$$

The asymptotic developments for $E_\pm(x,\lambda)$ together with (3.10) lead to an expansion for $\chi_F(\lambda)$. The $2N_\mathcal{E} \times 2N_\mathcal{E}$ matrix function $\chi_F(\lambda) = \chi_F(\omega^2)$ may be written as a sum,

$$\chi_F(\omega^2) = F_1(\omega) + F_J(\omega) + R(\omega), \tag{5.4}$$

with the first term being the entire 2π-periodic function

$$F_1(\omega) = M_1 + \exp(\mathrm{i}\omega)M_2,$$

whose properties are described in theorem 4.1, and for a fixed $J \geqslant 2$

$$F_1(\omega) + F_J(\omega) = (B_1 \ \ B_2)\begin{pmatrix} I_N & \zeta I_N \\ I_N & -\zeta I_N\end{pmatrix} + (B_3 \ \ B_4)\begin{pmatrix} E_{J,+}(\omega) & E_{J,-}(\omega) \\ E_{J,+}'(\omega) & E_{J,-}'(\omega)\end{pmatrix}\begin{pmatrix} I_N & 0_N \\ 0_N & \zeta I_N\end{pmatrix}. \tag{5.5}$$

From the definition of F_J and the more or less standard ([4, 14]) estimates for the remainder $R(\omega)$, one obtains the following lemma.

Lemma 5.1. *The functions $F_J(\omega)$ and $R(\omega)$ are analytic in the open half plane $\Re(\omega) > 0$. For $0 < \sigma_0 < \infty$ and $0 < \tau_0 < \infty$, let*

$$S_0 = \{\omega | \Re(\omega) > \sigma_0, |\Im(\omega)| < \tau_0\} \tag{5.6}$$

denote a closed horizontal strip in the right half plane. For $\omega \in S_0$

$$\|R(\omega)\| \leqslant C|\omega|^{-J},$$

and

$$\|F_J(\omega)\| \leqslant C_1|\omega|^{-1}.$$

5.2. Eigenvalue asymptotics

Let us summarize the main developments so far. The eigenvalues of $-D^2 + Q$ coincide with the roots of $\det(\chi_S(\lambda))$, and the geometric multiplicity of the eigenvalues agrees with the dimension of the null space of the matrix characteristic function $\chi_S(\lambda)$. Except for $\lambda = 0$, the dimension of the null space of $\chi_S(\lambda)$ agrees with the dimension of the null space of $\chi_F(\lambda)$, which has an expansion described in (5.2)–(5.5).

$F_1(\omega)$ is an entire 2π-periodic matrix function. Let $\omega_1 < \cdots < \omega_K$ denote the roots of $\det F_1(\omega)$ in the interval $(0, 2\pi]$, and let $m(k)$ denote the multiplicity of 0 as an eigenvalue of $F_1(\omega_k)$. The sum of the dimensions of the null spaces of $F_1(\omega)$ over a period is $2N_{\mathcal{E}}$. The function $F_1^{-1}(\omega)$ has simple poles at $\omega = \omega_k$. For integers $n \geqslant 0$ let $\omega_{k,n} = \omega_k + 2\pi n$. For $r_0 > 0$ define

$$D_{k,n} = \{|\omega - \omega_{k,n}| < r_0\}, \qquad \partial D_{k,n} = \{|\omega - \omega_{k,n}| = r_0\}.$$

Assume that r_0 is chosen small enough that the closed disks $\overline{D_{k,n}}$ are pairwise disjoint.

Lemma 5.2. *With S_0 as defined in (5.6), there are positive constants C and σ_1 such that $F_1 + F_J$ is invertible in*

$$[S_0 \cap \{|\Re(\omega)| \geqslant \sigma_1\}] \Big\backslash \Big[\bigcup_{k,n} B_{k,n}\Big], \qquad B_{k,n} = \{|\omega - \omega_{k,n}| \leqslant C|\omega_{k,n}|^{-1}\}.$$

Let $z_1, \ldots, z_J$ be the roots of $\det(F_1 + F_J)(z_j)$ *in $B_{k,n}$. Then the number of roots z_j, counted with multiplicity, is $m(k)$.*

Moreover, if r_0 is sufficiently small and $|z|$ is sufficiently large, $\det(F_1 + F_J)(z)$ *has a positive lower bound for $z \in \partial D_{k,n}$, independent of k and n.*

Proof. The function $F_1(\omega)$ is periodic, and for

$$\omega \in S_0 \Big\backslash \Big[\bigcup_{k,n} D_{k,n}\Big]$$

it is invertible, so the decay of $F_J(\omega)$ gives

$$\begin{aligned}\det(F_1 + F_J)(\omega) &= \det F_1(\omega) \det\left[I_N + F_1^{-1}(\omega)F_J(\omega)\right] \\ &= \det F_1(\omega)[1 + O(|\omega|^{-1})].\end{aligned} \tag{5.7}$$

If $\Re(\omega)$ is also sufficiently large, then

$$|\det(F_1 + F_J) - \det(F_1)| < |\det(F_1(\omega))|,$$

and by Rouche's theorem [16, p 152] the matrix function $F_1 + F_J$ is invertible in $S_0 \setminus \left[\bigcup_{k,n} D_{k,n} \right]$, and inside each disk $D_{k,n}$ the functions $\det(F_1 + F_J)$ and $\det(F_1)$ have the same number of zeros, which is $m(k)$.

These results now extend to $B_{k,n}$. Since $F_1^{-1}(\omega)$ has a simple pole at $\omega_k + 2n\pi$, and $F_1(\omega)$ is periodic with period 2π, there are positive constants $C_2, r_1 < r_0$ such that

$$\left\| F_1^{-1}(\omega - \omega_k - 2n\pi) \right\| \leqslant C_2 |\omega - \omega_k - 2n\pi|^{-1}, \qquad 0 < |\omega - \omega_k - 2n\pi| \leqslant r_1, \tag{5.8}$$

and this estimate holds independent of k and n.

Since

$$(F_1 + F_J)(\omega) = F_1(\omega)\left[I_N + F_1^{-1}(\omega) F_J(\omega) \right],$$

$F_1 + F_J$ is invertible if

$$\left\| F_1^{-1}(\omega) F_J(\omega) \right\| < 1.$$

By lemma 5.1 and (5.8) this estimate will hold for

$$0 < r_2 \leqslant |\omega - \omega_k - 2n\pi| \leqslant r_1$$

if

$$C_1 C_2 |\omega|^{-1} |\omega - \omega_k - 2n\pi|^{-1} < 1,$$

that is if

$$r_2 > C_1 C_2 |\omega|^{-1},$$

and the rest is clear. □

Suppose $X = [x_1, \dots, x_m]$ is an unordered m-tuple of complex numbers. By Newton's identities [17, p 208] the power sums

$$\sum_{i=1}^{m} x_i^p, \qquad p = 1, \dots, m,$$

uniquely determine X. Let $\gamma_{k,n}$ be a simple closed path traversing $\partial D_{k,n}$ once in the counterclockwise direction. A variant of Rouche's theorem [16, p 152] allows us to compare power sums coming from $F_1 + F_J$ with sums coming from χ_F.

Theorem 5.3. *For $i = 1, \dots, m(k)$ let z_i and w_i respectively be the roots of* $\det(F_1 + F_J)$ *and* $\det \chi_F$ *in $D_{k,n}$, with both sets of roots listed with multiplicity. Let $\omega_{k,n}$ be the root of* $\det(F_1)$ *in $D_{k,n}$. Then for $p \geqslant 1$*

$$\sum_{i=1}^{m(k)} (z_i - \omega_{k,n})^p - \sum_{i=1}^{m(k)} (w_i - \omega_{k,n})^p = O(|\omega|^{-J}).$$

Proof. With $f = \det(F_1 + F_J)$ the power sums

$$\sum_{i=1}^{m(k)} (z_i - \omega_{k,n})^p$$

are given by the integral formula [16, p 152]

$$\frac{1}{2\pi \mathrm{i}} \int_{\gamma_{k,n}} (\omega - \omega_{k,n})^p \frac{f'(\omega)}{f(\omega)} \, \mathrm{d}\omega.$$

As noted in lemma 5.2, $f(\omega)$ is bounded away from 0 uniformly on $\partial D_{k,n}$. By (5.7) and the Cauchy integral formula we may also conclude that $f'(\omega)$ is uniformly bounded on $\partial D_{k,n}$.

If $g = \det(\chi_F(\omega))$ the same boundedness assertions apply to g, and the difference of power sums is

$$\frac{1}{2\pi \mathrm{i}} \int_{\gamma_{k,n}} (\omega - \omega_{k,n})^p \left[\frac{f'(\omega)}{f(\omega)} - \frac{g'(\omega)}{g(\omega)} \right] \mathrm{d}\omega$$
$$= \frac{1}{2\pi \mathrm{i}} \int_{\gamma_{k,n}} (\omega - \omega_{k,n})^p \partial_\omega [\log(f(\omega)) - \log(g(\omega))] \, \mathrm{d}\omega$$
$$= \frac{1}{2\pi \mathrm{i}} \int_{\gamma_{k,n}} (\omega - \omega_{k,n})^p \partial_\omega \log\left(\frac{f(\omega)}{g(\omega)}\right) \mathrm{d}\omega.$$

Since the functions f and g are bounded away from 0 on $\partial D_{k,n}$, we also have

$$\frac{f}{g} = \frac{\det(F_1 + F_J)(\omega)}{\det(\chi_F(\omega))} = \det(I + O(|\omega|^{-J})), \qquad \omega \in \partial D_{k,n}.$$

We then see that $\log\left(\frac{f(\omega)}{g(\omega)}\right)$ is single valued and analytic on $\partial D_{k,n}$, so we may integrate by parts to get

$$\frac{1}{2\pi \mathrm{i}} \int_{\gamma_{k,n}} (\omega - \omega_{k,n})^p \partial_\omega \log\left(\frac{f(\omega)}{g(\omega)}\right) \mathrm{d}\omega = -\frac{1}{2\pi \mathrm{i}} \int_{\gamma_{k,n}} p(\omega - \omega_{k,n})^{p-1} \log\left(\frac{f(\omega)}{g(\omega)}\right) \mathrm{d}\omega.$$

The estimate

$$\log\left(\frac{f(\omega)}{g(\omega)}\right) = O(|\omega|^{-J}), \qquad \omega \in \partial D_{k,n},$$

and the uniformly bounded contour lengths give the claimed estimates. □

5.3. A spectral shift theorem

Our final result is a limit theorem for eigenvalue clusters, where as before $\omega_{k,n}^2$ is an eigenvalue for $-D^2$ on the graph, $\omega_{k,n} \in D_{k,n}$. As motivation, consider the periodic problem for $0 \leqslant x \leqslant 1$,

$$-y'' + p(x)y = \lambda y, \qquad y(0) = y(1), \qquad y'(0) = y'(1).$$

For large values of λ, there will be an eigenvalue pair $\lambda_{2n-1}, \lambda_{2n}$ located near $(2n\pi)^2$. Classical asymptotics [18, p 40] gives the estimate

$$\lim_{n\to\infty} (\lambda_{2n-1} + \lambda_{2n}) - 2(2n\pi)^2 = 2 \int_0^1 p(x) \, \mathrm{d}x.$$

This result has a known extension to spheres [19].

For quantum graphs with edges of length 1, we have the following generalization to cluster traces. Note that the sums computed below are slightly different from those of theorem 5.3.

Theorem 5.4. *Suppose w_i^2 are the eigenvalues of $-D^2 + q$, listed with multiplicity, with $w_i \in D_{k,n}$. Then*

$$\lim_{n\to\infty} \sum_{w_i \in D_{k,n}} \left(w_i^2 - \omega_{k,n}^2\right) = \Lambda_k(q),$$

where $\Lambda_k(q)$ is a linear combination of the numbers

$$\int_0^1 q_j(x) \, \mathrm{d}x, \qquad j = 1, \ldots, N_{\mathcal{E}}.$$

Proof. For this result, it suffices to use $J = 2$. Using (5.3) define

$$E_1 = \begin{pmatrix} \exp(\mathrm{i}\omega) I_N & \exp(-\mathrm{i}\omega) I_N \\ \exp(\mathrm{i}\omega) I_N & -\exp(-\mathrm{i}\omega) I_N \end{pmatrix}$$

and

$$E_2 = \begin{pmatrix} E_{J,+} & E_{J,-} \\ E'_{J,+} & E'_{J,-} \end{pmatrix} = E_1 + \frac{1}{2\mathrm{i}\omega} \begin{pmatrix} \exp(\mathrm{i}\omega)[Q] & -\exp(-\mathrm{i}\omega)[Q] \\ \exp(\mathrm{i}\omega)[Q] & \exp(-\mathrm{i}\omega)[Q] \end{pmatrix}. \tag{5.9}$$

Then

$$\begin{aligned} F_2(\omega) &= (B_3 \quad B_4)[E_2 - E_1] \begin{pmatrix} I_N & 0_N \\ 0_N & \zeta I_N \end{pmatrix} \\ &= \frac{1}{2\mathrm{i}\omega}(B_3 \quad B_4) \begin{pmatrix} \exp(\mathrm{i}\omega)[Q] & -\zeta \exp(-\mathrm{i}\omega)[Q] \\ \exp(\mathrm{i}\omega)[Q] & \zeta \exp(-\mathrm{i}\omega)[Q] \end{pmatrix} \\ &= \frac{1}{2\mathrm{i}\omega}(\zeta(B_3 + B_4)[Q] \quad (B_4 - B_3)[Q]). \end{aligned}$$

We want to calculate the asymptotics of the first two terms

$$\sum_i (w_i - \omega_{k,n}), \qquad \sum_i \left(w_i^2 - \omega_{k,n}^2\right).$$

With $\gamma_{k,n}$ parametrizing $\partial D_{k,n}$ and using a technique similar to that of theorem 5.3,

$$\begin{aligned} \sum_i \left(w_i^p - z_i^p\right) &= \frac{1}{2\pi \mathrm{i}} \int_{\gamma_{k,n}} \omega^p \partial_\omega \log\left(\frac{\det(\chi_F)}{\det(F_1 + F_2)}\right) \mathrm{d}\omega \\ &= -\frac{1}{2\pi \mathrm{i}} \int_{\gamma_{k,n}} p\omega^{p-1} \log\left(\frac{\det(\chi_F)}{\det(F_1 + F_2)}\right) \mathrm{d}\omega. \end{aligned}$$

From

$$\chi_F(\omega) = F_1 + F_2 + O(\omega^{-2}),$$

and the uniform bounds for $(F_1 + F_2)^{-1} = \left(I_{2N} + F_1^{-1} F_2\right)^{-1} F_1^{-1}$ on $\partial D_{k,n}$, it follows that

$$\begin{aligned} \frac{\det(\chi_F)}{\det(F_1 + F_2)}) &= \det((F_1 + F_2)^{-1} \chi_F) = \det(I_{2N} + O(\omega^{-2})) \\ &= 1 + O(\omega^{-2}), \qquad \omega \in \partial D_{k,n}. \end{aligned}$$

Since

$$\log\left(\frac{\det(\chi_F)}{\det(F_1 + F_2)}\right) = O(\omega^{-2}),$$

taking limits over the sums from $D_{k,n}$ as $n \to \infty$ gives

$$\lim_{n\to\infty} \sum_i \left(w_i^p - z_i^p\right) = 0, \qquad p = 1, 2, \tag{5.10}$$

and w_i may be replaced by z_i for $p = 1, 2$.

So for $p = 1, 2$ consider

$$\sum_i \left(z_i^p - \omega_{k,n}^p\right) = -\frac{1}{2\pi \mathrm{i}} \int_{\gamma_{k,n}} p\omega^{p-1} \log\left(\frac{\det(F_1 + F_2)}{\det(F_1)}\right) \mathrm{d}\omega.$$

Since

$$\log\det\left(I_{2N} + F_1^{-1} F_2\right) = O(\omega^{-1}),$$

and using (5.10), the $p = 1$ case has

$$\lim_{n\to\infty} \sum_{w_i\in D_{k,n}} (w_i - \omega_{k,n}) = \lim_{n\to\infty} \sum_{z_i\in D_{k,n}} (z_i - \omega_{k,n}) = 0.$$

Now suppose $p = 2$. First of all we note that $\det\left(I + F_1^{-1}F_2\right)$ is the product of the diagonal entries of $I_{2N} + F_1^{-1}F_2$ plus terms that are $O(\omega^{-2})$ on $\partial D_{k,n}$. These terms contribute 0 to the limit being computed. Expanding the product of the diagonal entries $\prod(1+d_{rr})$, with $d_{rr} = O(\omega^{-1})$, we find

$$\det\left(I_{2N} + F_1^{-1}F_2\right) = 1 + \mathrm{tr}\left(F_1^{-1}F_2\right) + O(\omega^{-2}), \qquad \omega \in \partial D_{k,n}.$$

Similarly

$$\log\det\left(I_{2N} + F_1^{-1}F_2\right) = \mathrm{tr}\left(F_1^{-1}F_2\right) + O(\omega^{-2}), \qquad \omega \in \partial D_{k,n}.$$

Thus, with the help of (5.10),

$$\begin{aligned}\lim_{n\to\infty} \sum_{w_i\in D_{k,n}} \left(w_i^2 - \omega_{k,n}^2\right) &= \lim_{n\to\infty} \sum_{z_i\in D_{k,n}} \left(z_i^2 - \omega_{k,n}^2\right)\\ &= -\lim_{n\to\infty} \frac{1}{2\pi\mathrm{i}} \int_{\gamma_{k,n}} 2\,\mathrm{tr}\left(F_1^{-1}\omega F_2\right) \mathrm{d}\omega\\ &= -\lim_{n\to\infty} \frac{1}{2\pi} \int_{\gamma_{k,n}} \mathrm{tr}\, F_1^{-1}(\zeta(B_3 + B_4)[Q] \quad (B_4 - B_3)[Q])\,\mathrm{d}\omega.\end{aligned} \tag{5.11}$$

The result is finished by noting that the integrand is periodic in ω with period 2π, so the integrals are independent of n. □

We conclude with some remarks about higher order generalizations of theorem 5.4. For $J > 2$ let $z_i(J)$ denote the roots of $\det(F_1 + F_J)$, which are located in $D_{k,n}$. As in the proof above, there is an error estimate

$$\lim_{n\to\infty} \sum_i \left(w_i^p - z_i^p(J)\right) = 0, \qquad p = 1, 2, \ldots, J.$$

Assuming the limits exist, it follows that

$$\lim_{n\to\infty} \sum_i \left(w_i^p - z_i^p(J-1)\right) = \lim_{n\to\infty} \sum_i \left(z_i^p(J) - z_i^p(J-1)\right), \qquad p = 1, 2, \ldots, J.$$

The differences of powers on the right are represented by

$$\sum_i \left(z_i^p(J) - z_i^p(J-1)\right) = -\frac{1}{2\pi\mathrm{i}} \int_{\gamma_{k,n}} p\omega^{p-1} \log\left(\frac{\det(F_1 + F_J)}{\det(F_1 + F_{J-1})}\right) \mathrm{d}\omega. \tag{5.12}$$

The function $\det(F_1 + F_J)/\det(F_1 + F_{J-1})$ has two convenient representations. First,

$$\begin{aligned}\frac{\det(F_1 + F_J)}{\det(F_1 + F_{J-1})} &= \det(I_{2N} + (F_1 + F_{J-1})^{-1}(F_J - F_{J-1}))\\ &= 1 + O(\omega^{J-1}), \qquad \omega \in \partial D_{k,n}.\end{aligned}$$

In particular, (5.12) gives

$$\lim_{n\to\infty} \sum_i \left(w_i^p - z_i^p(J-1)\right) = 0 \qquad p = 1, 2, \ldots, J-1.$$

Alternatively,

$$\frac{\det(F_1 + F_J)}{\det(F_1 + F_{J-1})} = \frac{\det\left(I_{2N} + F_1^{-1}F_J\right)}{\det\left(I_{2N} + F_1^{-1}F_{J-1}\right)}.$$

The matrix function $\left[I_{2N} + F_1^{-1}F_{J-1}\right]^{-1}(\omega)$ has a geometric series expansion, allowing us to find an 'elementary' representative for the order ω^{J-1} term of $\log(\det(F_1+F_J)/\det(F_1+F_{J-1})$, and thus a formula in the style of (5.11).

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