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Spectral averaging techniques for Jacobi matrices with matrix entries

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Abstract

A Jacobi matrix with matrix entries is a self-adjoint block tridiagonal matrix with invertible blocks on the off-diagonals. Averaging over boundary conditions leads to explicit formulae for the averaged spectral measure which can potentially be useful for spectral analysis. Furthermore, another variant of spectral averaging over coupling constants for these operators is presented.

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1. Introduction

Many variants of spectral averaging for one-dimensional Sturm–Liouville or Jacobi operators are known [CL]. If such operators depend on some continuous parameters, then the spectral averaging principle states that the spectral measures averaged over these parameters with respect to a measure with density are themselves absolutely continuous. In refinements useful for a detailed spectral analysis, it is possible to prove that they are even equivalent to the Lebesgue measure [dRT, dRMS]. The continuous parameters are typically boundary conditions or coupling constants.

In this work, we are focussing on generalizations of these spectral averaging results to Jacobi matrices with matrix entries which are in the limit-point case. We expect them readily to carry over to Hamiltonian systems [HS] and Dirac finite difference operators [CGR]. Standard references on Jacobi matrices with matrix entries are [Ber, Sak], but we will follow closely the notations of our recent works [SB1, SB2]. The only prior contribution to spectral averaging for these operators seems to be due to Carmona and Lacroix [CL]. Unfortunately, their work does not give all the details of proof and the presentation is not conceptually structured nor does it cover full generality. Part of this work, in particular theorem 2, is thought to fill these gaps. The main ingredient of the proof is the Cauchy formula for integration over the unitary group as proven by Hua [Hua] (it is recalled in an appendix). Theorem 2 leads to a formula (stated in theorem 3) establishing a close link between spectral properties of the Jacobi operators in the limit point case and their formal solutions expressed in terms of the transfer matrices. We believe that theorem 3 can potentially be a useful alternative tool (other than

Kotani theory [KS]) for proving existence of absolutely continuous spectrum. Finally, theorem 4 provides a matrix version of a well-known identity of rank one perturbation theory, showing that averaging of the spectral measure over both boundary conditions leads to the Lebesgue measure. As an application, spectral stability results with respect to local perturbations are presented. It is shown that also averages over fewer parameters than the whole set of boundary conditions lead to averaged spectral measures which are equivalent to the Lebesgue measure, at least locally in energy. This last part generalize the results in [dRMS]. As we lack a subordinacy theory for Jacobi matrices with matrix entries the applications to spectral theory of that paper do not carry over.

This work complements our prior works [SB1] on Sturm–Liouville oscillation theory and [SB2] on Weyl theory for Jacobi matrices with matrix entries. Heavy use is being made of the matrix Möbius transformation on which there is an abundant literature (see references therein), but the main facts relevant for the present purposes are resembled in an appendix and all their short proofs are given in [SB1, SB2].

2. Setup and review of needed results

Notations. The matrix entries of the Jacobi matrices are of size $L \in \mathbb{N}$. Matrices of size $L \times L$ are denoted by roman letters, those of size $2L \times 2L$ by calligraphic ones. The upper half-plane $\mathbb{U}_L$ is the set of complex $L \times L$ matrices satisfying $\imath(Z^* - Z) > \mathbf{0}$. Its closure $\overline{\mathbb{U}_L}$ is given by matrices satisfying $\imath(Z^* - Z) \geqslant \mathbf{0}$. The boundary is a stratified space $\partial\mathbb{U}_L = \cup_{l=1}^{L} \partial_l \mathbb{U}_L$, where $\partial_l \mathbb{U}_L$ contains those matrices in $\overline{\mathbb{U}_L}$ for which the kernel of $Z^* - Z$ is l-dimensional.

2.1. The Jacobi matrix and its resolvent

Fix two integers $L, N \in \mathbb{N}$ and let $(T_n)_{n=2,\ldots,N}$ and $(V_n)_{n=1,\ldots,N}$ be sequences of respectively invertible and self-adjoint $L \times L$ matrices with complex entries. Furthermore let the left and right boundary conditions $\hat{Z}$ and Z be also self-adjoint $L \times L$ matrices. Then the associated Jacobi matrix with matrix entries $H^N_{\hat{Z},Z}$ is by definition the self-adjoint operator acting on states $\phi = (\phi_n)_{n=1,\ldots,N} \in \ell^2(1,\ldots,N) \otimes \mathbb{C}^L$ by

$$\left(H^N_{\hat{Z},Z}\phi\right)_n = T_{n+1}\phi_{n+1} + V_n\phi_n + T_n^*\phi_{n-1}, \qquad n = 1,\ldots,N, \tag{1}$$

where $T_1 = T_{N+1} = \mathbf{1}$, together with the boundary conditions

$$\phi_0 = \hat{Z}\phi_1, \qquad \phi_{N+1} = -Z\phi_N. \tag{2}$$

If $\hat{Z} = \mathbf{0}$ and $Z = \mathbf{0}$, one speaks of Dirichlet boundary conditions at the left and right boundaries respectively. It will be useful to allow also non-selfadjoint boundary conditions $\hat{Z}, Z \in \overline{\mathbb{U}_L}$ hence giving rise to a possibly non-selfadjoint operator $H^N_{\hat{Z},Z}$. One can rewrite $H^N_{\hat{Z},Z}$ as an $NL \times NL$ matrix with $L \times L$ block entries:

$$H^N_{\hat{Z},Z} = \begin{pmatrix} V_1 - \hat{Z} & T_2 & & & & \\ T_2^* & V_2 & T_3 & & & \\ & T_3^* & V_3 & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & V_{N-1} & T_N \\ & & & & T_N^* & V_N - Z \end{pmatrix}. \tag{3}$$

At times, our interest will only be in the dependence of the right boundary condition Z, and then the index $\hat{Z}$ will be suppressed.

As for a one-dimensional Jacobi matrix, it is useful to rewrite the eigenvalue equation

$$\left(H^N_{\hat{Z},Z}\phi\right)_n = z\phi_n, \qquad n = 1, \dots, N, \tag{4}$$

for a complex energy $z \in \mathbb{C}$ in terms of the $2L \times 2L$ transfer matrices $\mathcal{T}^z_n$ defined by

$$\mathcal{T}^z_n = \begin{pmatrix} (z\mathbf{1} - V_n)T_n^{-1} & -T_n^* \\ T_n^{-1} & \mathbf{0} \end{pmatrix}, \qquad n = 1, \dots, N, \tag{5}$$

namely

$$\begin{pmatrix} T_{n+1}\phi_{n+1} \\ \phi_n \end{pmatrix} = \mathcal{T}^z_n \begin{pmatrix} T_n\phi_n \\ \phi_{n-1} \end{pmatrix}, \qquad n = 1, \dots, N. \tag{6}$$

This gives a solution of the eigenvalue equation (4) which, however, does not necessarily satisfy the boundary condition (2). Now $z \in \mathbb{C}$ is an eigenvalue of $H^N_{\hat{Z},Z}$ if and only if there is a solution of (4), that is produced by (6), which satisfies (2). As is well established, one can understand (2) as requirement on the solution at sites 0, 1 and N, $N+1$ respectively to lie in L-dimensional planes in $\mathbb{C}^{2L}$. The corresponding two planes are described by the two $2L \times L$ matrices (one thinks of the L columns as spanning the plane)

$$\hat{\Phi}_{\hat{Z}} = \begin{pmatrix} \mathbf{1} \\ -\hat{Z} \end{pmatrix}, \qquad \Phi_Z = \begin{pmatrix} -Z \\ \mathbf{1} \end{pmatrix}. \tag{7}$$

Then the boundary conditions (2) can be rewritten as

$$\begin{pmatrix} T_1\phi_1 \\ \phi_0 \end{pmatrix} \in \hat{\Phi}_{\hat{Z}}\mathbb{C}^L, \qquad \begin{pmatrix} T_{N+1}\phi_{N+1} \\ \phi_N \end{pmatrix} \in \Phi_Z\mathbb{C}^L. \tag{8}$$

One way to attack the eigenvalue problem is to consider the L-dimensional plane $\hat{\Phi}_{\hat{Z}}$ as the initial condition for an evolution of L-dimensional planes under the application of the transfer matrices:

$$\Phi^z_n = \mathcal{T}^z_n\Phi^z_{n-1}, \qquad \Phi^z_0 = \hat{\Phi}_{\hat{Z}}. \tag{9}$$

Because the transfer matrices are invertible, this produces an L-dimensional set of solutions of (6). With the correspondence

$$\Phi^z_n = \begin{pmatrix} T_{n+1}\phi^z_{n+1} \\ \phi^z_n \end{pmatrix}, \tag{10}$$

this also gives a matricial solution ϕ^z_n of (4). Due to the initial condition in (9) the left boundary condition at sites 0, 1 is automatically satisfied. The dimension of the intersection of the plane Φ^z_N with the plane Φ_Z gives the number of linearly independent solutions of (4) at energy z, and therefore the multiplicity of z as eigenvalue of $H^N_{\hat{Z},Z}$.

Given (9), but also its own sake, it is natural to introduce the transfer matrices over several sites by

$$\mathcal{T}^z(n,m) = \mathcal{T}^z_n \cdot \ldots \cdot \mathcal{T}^z_{m+1}, \qquad n > m, \tag{11}$$

as well as $\mathcal{T}^z(n,n) = \mathbf{1}$ and $\mathcal{T}^z(n,m) = \mathcal{T}^z(m,n)^{-1}$ for $n < m$. With this notation, the solution of the eigenvalue equation (4) satisfies $\Phi^z_n = \mathcal{T}^z(n,m)\Phi^z_m$ and, in particular,

$\Phi_n^z = \mathcal{T}^z(n,0)\hat{\Phi}_{\hat{Z}}$. Of particular importance will be the transfer matrix $\mathcal{T}^z(N,0)$ across the whole sample. Let us introduce the notations

$$\mathcal{T}^z(N,0) = \begin{pmatrix} A_N^z & B_N^z \\ C_N^z & D_N^z \end{pmatrix}, \tag{12}$$

where all entries are $L \times L$ matrices. These matrices will intervene in many of the results below. Let us point out that $\mathcal{T}^z(N,0)$ and all its entries do not depend on the boundary conditions $\hat{Z}$ and Z. The transfer matrix including boundary conditions is then

$$\begin{pmatrix} \mathbf{1} & Z \\ \mathbf{0} & \mathbf{1} \end{pmatrix} \mathcal{T}^z(N,0) \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ -\hat{Z} & \mathbf{1} \end{pmatrix} = \begin{pmatrix} A_N^z + ZC_N^z - B_N^z\hat{Z} - ZD_N^z\hat{Z} & B_N^z + ZD_N^z \\ C_N^z - D_N^z\hat{Z} & D_N^z \end{pmatrix}. \tag{13}$$

Now we introduce the resolvent. Let $\pi_n : \mathbb{C}^L \to \mathbb{C}^{NL}$ for $n = 1, \ldots, N$ denote the partial isometry

$$\pi_n|l\rangle = |n, l\rangle, \qquad l = 1, \ldots, L,$$

where the Dirac notation for localized states in $\mathbb{C}^N \otimes \mathbb{C}^L$ is used. Then the $L \times L$ Green's matrix is given by

$$G_N^z(\hat{Z}, Z, n, m) = \pi_n^* \big(H_{\hat{Z},Z}^N - z\mathbf{1}\big)^{-1} \pi_m.$$

Proposition 1. *([SB2]). For $\hat{Z}, Z \in \overline{\mathbb{U}_L}$,*

$$\begin{aligned} G_N^z(\hat{Z}, Z, 1, 1) &= \big[A_N^z + ZC_N^z - B_N^z\hat{Z} - ZD_N^z\hat{Z}\big]^{-1}\big[B_N^z + ZD_N^z\big] \\ &= \big[\big[A_N^{\overline{z}} + ZC_N^{\overline{z}} - B_N^{\overline{z}}\hat{Z} - ZD_N^{\overline{z}}\hat{Z}\big]^{-1}\big[B_N^{\overline{z}} + ZD_N^{\overline{z}}\big]\big]^*. \end{aligned}$$

2.2. Parametrization of the boundary conditions

The underlying Hermitian symplectic structure is an important ingredient in most of the equations of the last sections, in particular in their proofs. It is necessary in order to understand what the adequate spectral averaging over the boundary conditions is. This section first recalls basic fact about the symplectic structure, which will then be applied below. Let the symplectic form $\mathcal{J}$ be the $2L \times 2L$ matrix defined by

$$\mathcal{J} = \begin{pmatrix} 0 & -\mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}.$$

An L-dimensional plane described by a $2L \times L$ matrix Φ of maximal rank is called Lagrangian (or also isotropic, or simply symplectic) if $\Phi^*\mathcal{J}\Phi = \mathbf{0}$.

Two L-dimensional planes described by $2L \times L$ matrices Φ and Ψ are called equivalent if there exists $c \in \mathrm{Gl}\,(L, \mathbb{C})$ with $\Phi = \Psi c$. The Lagrangian Grassmannian $\mathbb{L}_L$ is by definition the set of equivalence classes of Lagrangian planes. It is difficult to track back the original reference for the following result (it probably predates [Bot]). A short proof can be found in [SB1] where it is also shown how two natural symmetries are implemented.

Proposition 2. *The Lagrangian Grassmannian $\mathbb{L}_L$ is identified with the unitary group $\mathrm{U}(L)$ via the real analytic diffeomorphism $\Pi : \mathbb{L}_L \to \mathrm{U}(L)$ given by*

$$\Pi([\Phi]_\sim) = (a - \imath b)(a + \imath b)^{-1}, \qquad \Phi = \begin{pmatrix} a \\ b \end{pmatrix}.$$

Due to this theorem there is a natural measure on the Lagrangian Grassmannian $\mathbb{L}_L^{\mathbb{C}}$ given by the pull-back under Π of the Haar measure on the unitary group.

The Lie group conserving the (Hermitian) symplectic structure is the (Hermitian) symplectic group SP $(2L, \mathbb{C})$ defined by those $2L \times 2L$ matrices $\mathcal{T}$ satisfying $\mathcal{T}^*\mathcal{J}\mathcal{T} = \mathcal{J}$. Clearly, if Φ describes a Lagrangian plane, then so does $\mathcal{T}\Phi$ for any $\mathcal{T} \in$ SP $(2L, \mathbb{C})$. Isomorphic to the Hermitian symplectic group is the Lorentz group of signature (L, L) defined by $\mathrm{U}(L, L, \mathbb{C}) = \mathcal{C}$ SP $(2L, \mathbb{C})\mathcal{C}^*$, where $\mathcal{C}$ is the Cayley transformation introduced as the matrix

$$\mathcal{C} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1} & -\imath\mathbf{1} \\ \mathbf{1} & \imath\mathbf{1} \end{pmatrix}.$$

Next let us exhibit explicitly the symplectic structure in the equations of section 2.1. Both of the planes $\hat{\Phi}_{\hat{Z}}$ and Φ_Z used as boundary conditions in (8) are Lagrangian in the above sense. Actually there are many Lagrangian planes which cannot be written in this way, but they form a set of zero measure. Due to proposition 2, it is natural to identify the left and right boundary conditions with unitary matrices:

$$\hat{U} = \Pi([\hat{\Phi}_{\hat{Z}}]_\sim), \qquad U = \Pi([\Phi_Z]_\sim). \tag{14}$$

In other terms, this means $U = \mathcal{C} \cdot (-Z)$ and $\hat{U} = -\mathcal{C} \cdot \hat{Z}$. Furthermore, let us set

$$U_n^E = \Pi([\Phi_n^E]_\sim),$$

where Φ_n^E is the solution (9) which automatically satisfies the left boundary condition. Then $U_0^E = \hat{U}$. Using the correspondence (14), we also set

$$G_N^z(\hat{U}, U) = G_N^z(\hat{Z}, Z, 1, 1)\ .$$

As $z \mapsto G_N^z(\hat{U}, U) \in \mathbb{U}_L$ is analytic in z for $\mathrm{Imm}(z) > 0$, the Herglotz representation theorem [GT] associates a matrix-valued (averaged spectral) measure:

$$G_N^z(\hat{U}, U) = \int \rho_{\hat{U},U}^N(\mathrm{d}E) \frac{1}{E - z}.$$

2.3. The oscillation theorem

The oscillation theorem is another application of the parametrization of boundary conditions. It is stated for the sake of completeness and because it will be used in the proof of the result of section 4. Due to section 2.2, $E \in \mathbb{R} \mapsto \Phi_N^E$ is a path of Lagrangian planes and for each E the dimension of its intersection with the right boundary condition Φ_Z is the multiplicity of E as an eigenvalue of $H_{\hat{Z},Z}^N$. This intersection number was introduced by Bott [Bot] precisely for the study of the eigenvalue calculation of Sturm–Liouville operators, the continuous analogues of Jacobi matrices. Later on it was rediscovered by Maslov and a detailed survey of its properties is included in [SB1]. The intersection number can be conveniently calculated using the associated unitary U_N^E and this leads to the following theorem which was proven in [SB1] under the supplementary hypothesis that T_n's are positive, but the proof directly transposes to the slightly generalized situation considered here.

Theorem 1. *Let $E \in \mathbb{R}$, $N \geqslant 2$, and (for the sake of simplicity) the right boundary condition be Dirichlet, that is $Z = \mathbf{0}$. Then there are L strictly increasing real analytic functions $\theta_{N,l}^E : \mathbb{R} \to \mathbb{R}, l = 1, \ldots, L$, such that $\mathrm{e}^{\imath\theta_{N,l}^E}$ are the eigenvalues of U_N^E. The multiplicity of E as an eigenvalue of $H_{\hat{Z},\mathbf{0}}^N$ is equal to the multiplicity of -1 as an eigenvalue of U_N^E. Furthermore, the matrix $\frac{1}{\imath}(U_N^E)^* \partial_E U_N^E$ is positive definite.*

2.4. Limit point operators

If in the prior sections $N = \infty$, then the right boundary condition Z is pushed to infinity. If this gives a well-defined (essentially self-adjoint) operator $H_{\hat{Z}}$, one speaks of the limit point case. Various criteria for this can be given, the simplest one being that $\|T_n\|$ is uniformly bounded from below. Otherwise one needs the infinite operator having non-vanishing deficiency spaces and one has to consider various self-adjoint extensions. Here we restrict ourselves to limit point operators. For these operators, limits

$$G^z(\hat{U}) = \lim_{N\to\infty} G^z_N(\hat{U}, U)$$

exist, are independent of U and are the Green function of $H_{\hat{Z}}$. Its spectral measure is denoted by $\rho_{\hat{U}}$ and obtained as the weak limit of $\rho^N_{\hat{U},U}$.

3. Average over boundary conditions

Let us write $\mathrm{d}U$ for the normalized Haar measure on $\mathrm{U}(L)$.

Theorem 2. *For* $\mathrm{Im}m(z) > 0$, *one has*

$$\int \mathrm{d}U\, G^z_N(\mathbf{1}, U) = \left[A^z_N + \imath C^z_N\right]^{-1}\left[B^z_N + \imath D^z_N\right] \tag{15}$$

$$= \left[\left(B^{\bar{z}}_N\right)^* + \imath\left(D^{\bar{z}}_N\right)^*\right]\left[\left(A^{\bar{z}}_N\right)^* + \imath\left(C^{\bar{z}}_N\right)^*\right]^{-1}. \tag{16}$$

Moreover, for $E = \mathrm{Re}e(z)$, *and setting* $\mathrm{Im}m(A) = \frac{1}{2\imath}(A - A^*)$ *for any square matrix* A,

$$\lim_{\mathrm{Im}m(z)\downarrow 0} \int \mathrm{d}U\, \mathrm{Im}m\left(G^z_N(\mathbf{1}, U)\right) = \left[\left(A^E_N\right)^* A^E_N + \left(C^E_N\right)^* C^E_N\right]^{-1}. \tag{17}$$

Remark 1. A formula similar to (17) can be found in [CL], but the latter authors use the average over the Haar measure on the symmetric space of symmetric unitaries instead of the group $\mathrm{U}(L)$ (moreover, their proof seems to have several gaps).

Remark 2. It is easy to incorporate the left boundary condition $\hat{U} \neq \mathbf{1}$ using (13).

Remark 3. One way to define the closed Weyl disc $\overline{\mathbb{W}^z_N}$ is as the image of the map $Z \in \overline{\mathbb{U}_L} \mapsto G^z_N(\mathbf{1}, Z, 1, 1)$. As proven in [SB2] the points in the Weyl disc can also be parametrized by $G^z_N(\mathbf{1}, Z, 1, 1) = S^z_N + \left(R^z_N\right)^{\frac{1}{2}} W \left(R^{\bar{z}}_N\right)^{\frac{1}{2}}$, where S^z_N and $R^z_N > 0$ are properly defined center and radial operators, and $W \in \mathrm{U}(L)$ depends on Z, cf [SB2]. Taking the average over W with respect to to the Haar measure in this representation immediately gives $\int \mathrm{d}W\, G^z_N(\mathbf{1}, Z, 1, 1) = S^z_N$, which is *not* equal to the rhs of (15). The Jacobian of the change of variables $Z \mapsto W$ does not seem to be known (nor be of great importance).

Proof of theorem 2. First let us note that one can use the Möbius transformation to express $U = \Pi([\Phi_Z]_\sim) = \mathcal{C} \cdot (-Z)$. Hence also $Z = -\mathcal{C}^* \cdot U$. Starting from proposition 1, one therefore has

$$\int \mathrm{d}U\, G^z_N(\mathbf{1}, U) = \int \mathrm{d}U \left(A^z_N - \mathcal{C}^* \cdot U C^z_N\right)^{-1}\left(B^z_N - \mathcal{C}^* \cdot U D^z_N\right).$$

By (B.2),

$$\int \mathrm{d}U\, G^z_N(\mathbf{1}, U) = \int \mathrm{d}U \left(A^z_N + \mathcal{C}^* \cdot U C^z_N\right)^{-1}\left(B^z_N + \mathcal{C}^* \cdot U D^z_N\right).$$

(Alternatively to this argument, one could have defined the average on the lhs by the rhs.) In order to be able to apply the Cauchy formula (B.1) for $Z = \mathbf{0}$, it is sufficient to show the analyticity of the function

$$f(Z) = \left(A_N^z + \mathcal{C}^* \cdot ZC_N^z\right)^{-1}\left(B_N^z + \mathcal{C}^* \cdot ZD_N^z\right),$$

on the unit disc $\mathbb{D}_L^{\mathbb{C}}$ as well as its continuity on the closure $\overline{\mathbb{D}_L^{\mathbb{C}}}$ (strictly speaking, one should consider the entries of the matrix-valued function f). This follows from Weyl theory [SB2] combined with the fact that $(-\mathcal{C}^* \cdot Z)$ is in the closed lower half plane (for $Z \in \overline{\mathbb{D}_L^{\mathbb{C}}}$). The Cauchy formula (B.1) for $Z = \mathbf{0}$ now concludes the proof of (15) because $\mathcal{C}^* \cdot \mathbf{0} = \imath\mathbf{1}$. Formula (16) is proven similarly from the second identity in proposition 1.

It follows from the results of [SB2] that $A_N^z + \imath C_N^z = \left(A_N^z (C_N^z)^{-1} + \imath\mathbf{1}\right)C_N^z$ is invertible. Inserting $\mathbf{1} = [\left(A_N^z + \imath C_N^z\right)^*]^{-1}\left(A_N^z + \imath C_N^z\right)^*$ in (15) shows

$$\int \mathrm{d}U\, G_N^z(\mathbf{1}, U) = \left[\left(A_N^z\right)^* A_N^z + \left(C_N^z\right)^* C_N^z + \imath\left(\left(A_N^z\right)^* C_N^z - \left(C_N^z\right)^* A_N^z\right)\right]^{-1}$$
$$\left[\left(A_N^z\right)^* B_N^z + \left(C_N^z\right)^* D_N^z + \imath\left(\left(A_N^z\right)^* D_N^z - \left(C_N^z\right)^* B_N^z\right)\right].$$

As the transfer matrices at real energies are symplectic, the limit of vanishing imaginary part in the energy can be taken in this equation and that directly implies

$$\lim_{\mathrm{Im}m(z)\downarrow 0} \int \mathrm{d}U\, G_N^z(\mathbf{1}, U) = \left[\left(A_N^E\right)^* A_N^E + \left(C_N^E\right)^* C_N^E\right]^{-1}$$
$$\left[\left(A_N^E\right)^* B_N^E + \left(C_N^E\right)^* D_N^E + \imath\mathbf{1}\right],$$

where we used the identity $\left(A_N^E\right)^* D_N^E + \left(C_N^E\right)^* B_N^E = \mathbf{1}$ holding for any symplectic matrix. The same calculation can be carried out starting from (16) and adding the results up gives (17).

□

One corollary of theorem 2 is the following formula which links the averaged spectral measure defined by

$$\rho_{\hat{U}}^N = \int \mathrm{d}U\, \rho_{\hat{U},U}^N \tag{18}$$

to properties of the eigenfunctions of the transfer matrices at real energies.

Corollary 1. *For any* $E_0 < E_1$,

$$\frac{1}{2}\left[\rho_{\hat{U}}^N([E_0, E_1]) + \rho_{\hat{U}}^N((E_0, E_1))\right]$$
$$= \int_{E_0}^{E_1} \mathrm{d}E\left[|A_N^E - B_N^E\mathcal{C}^* \cdot (-\hat{U})|^2 + |C_N^E - D_N^E\mathcal{C}^* \cdot (-\hat{U})|^2\right]^{-1}.$$

In the limit point case, the averaging in (18) becomes irrelevant because $\rho_{\hat{U},U}^N$ converges weakly to the spectral measure $\rho_{\hat{U}}$ of $H_{\hat{Z}}$ as $N \to \infty$. This leads to the following formula for the spectral measure, which was already obtained by Carmona in the strictly one-dimensional case $L = 1$, and by Pearson [Pea] for one-dimensional Schrödinger operators. For the sake of simplicity, let us set $\hat{U} = \mathbf{1}$ so that $\mathcal{C}^* \cdot (-\hat{U}) = 0$.

Theorem 3. *Let the semi-infinite Jacobi matrix H be in the limit point case. Then, for any* $E_0 < E_1$,

$$\frac{1}{2}\left[\rho_{\mathbf{1}}([E_0, E_1]) + \rho_{\mathbf{1}}((E_0, E_1))\right] = \lim_{N\to\infty} \int_{E_0}^{E_1} \mathrm{d}E\left[\left(A_N^E\right)^* A_N^E + \left(C_N^E\right)^* C_N^E\right]^{-1}. \tag{19}$$

In the case where H is not in the limit point case, but has equal deficiency indices $n_+ = n_-$, the von Neumann theory provides us with a family of self-adjoint extensions indexed by the unitary group of dimension $n_+ = n_-$. Averaging the spectral measures over this unitary group (with an adequate density which can be deduced from theorem 6 of [SB2]) gives an averaged spectral measure which is given by the rhs of (19).

Next we also average over the left boundary condition $\hat{U}$. The associated averaged spectral measure is equal to the Lebesgue measure, a fact also known from the case $L = 1$.

Theorem 4. *For any N and H^N,*

$$4\int \mathrm{d}\hat{U}\,(\hat{U} - \mathbf{1})^{-1}\rho^N_{\hat{U}}(\mathrm{d}E)(\hat{U}^* - \mathbf{1})^{-1} = \mathbf{1}\,\mathrm{d}E. \tag{20}$$

The proof of the theorem is based on the following integral identity.

Lemma 1. *Let $0 < \mathcal{T} \in \mathrm{U}(L, L)$ and $V \in \mathrm{U}(L)$. Then*

$$\int \mathrm{d}U \left[\begin{pmatrix} U \\ V \end{pmatrix}^* \mathcal{T} \begin{pmatrix} U \\ V \end{pmatrix} \right]^{-1} = \mathbf{1}.$$

Proof. Let I denote the integral appearing in the lemma. First let us use that $0 < \mathcal{T} \in \mathrm{U}(L, L)$ can be transformed into a normal form by $\mathcal{M} = \begin{pmatrix} W & 0 \\ 0 & W' \end{pmatrix} \in \mathrm{U}(L, L) \cap \mathrm{U}(2L) \cong \mathrm{U}(L) \oplus \mathrm{U}(L)$ where $W, W' \in \mathrm{U}(L)$, namely

$$\mathcal{M}^*\mathcal{T}\mathcal{M} = \begin{pmatrix} \cosh(\eta) & \sinh(\eta) \\ \sinh(\eta) & \cosh(\eta) \end{pmatrix},$$

where $\eta = \mathrm{diag}(\eta_1, \ldots, \eta_L)$ is a diagonal matrix with non-negative entries. Let us denote the rhs by $\mathcal{T}_\eta$. Replacing this identity, one obtains

$$I = (W'V)^* \int \mathrm{d}U \left[\begin{pmatrix} WU(W'V)^* \\ \mathbf{1} \end{pmatrix}^* \mathcal{T}_\eta \begin{pmatrix} WU(W'V)^* \\ \mathbf{1} \end{pmatrix} \right]^{-1} (W'V),$$

so that using the invariance of the Haar measure $\mathrm{d}U$ one realizes that it is sufficient to consider the case $V = \mathbf{1}$ and $\mathcal{T} = \mathcal{T}_\eta$. First suppose $\eta > 0$. In this case, $\sinh(\eta)$ is invertible and

$$\begin{aligned} I &= \int \mathrm{d}U \big[\cosh(\eta)U + U\cosh(\eta) + U\sinh(\eta)U + \sinh\eta\big]^{-1} U \\ &= \int \mathrm{d}U \left[\left(U + \frac{\cosh(\eta) + \mathbf{1}}{\sinh(\eta)} \right)^{-1} \big(\sinh(\eta)\big)^{-1} \left(U + \frac{\cosh(\eta) - \mathbf{1}}{\sinh(\eta)} \right)^{-1} U \right]. \end{aligned}$$

To simplify notations, define $\alpha = \frac{\cosh(\eta)+\mathbf{1}}{\sinh(\eta)}$ and $\beta = \frac{\cosh(\eta)-\mathbf{1}}{\sinh(\eta)}$. Note that $0 < \beta < \mathbf{1} < \alpha$, $\alpha\beta = \mathbf{1}$ and $(\alpha - \beta)\sinh(\eta) = 2$. Now using

$$\int \mathrm{d}U (U + \beta)^{-1} U = \int \mathrm{d}U \sum_{n \geqslant 0} \big(- U^{-1}\beta\big)^n = \mathbf{1}, \qquad \int \mathrm{d}U (U + \alpha)^{-1} U = 0,$$

one gets with the resolvent identity

$$\begin{aligned} I - \mathbf{1} &= 2\int \mathrm{d}U \big[\big((U + \alpha)^{-1} - (\alpha - \beta)^{-1}\big)\sinh(\eta)^{-1}(U + \beta)^{-1} U\big] \\ &= -\int \mathrm{d}U (U + \alpha)^{-1} U = 0, \end{aligned}$$

and the proof is complete in the case $\eta > 0$. By continuity of the integral one also recovers the case $\eta \geqslant 0$.

□

Proof of theorem 4. This is based on corollary 1. Actually it is sufficient to show that the average of the integrand on the rhs of corollary 1 satisfies

$$4 \int \mathrm{d}\hat{U}\,(\hat{U} - \mathbf{1})^{-1}\big[|A_N^E - B_N^E \mathcal{C}^* \cdot (-\hat{U})|^2 + |C_N^E - D_N^E \mathcal{C}^* \cdot (-\hat{U})|^2\big]^{-1}(\hat{U}^* - \mathbf{1})^{-1} = \mathbf{1}.$$

(Note that the various inverse appearing in this formula do not exist on a set of zero measure.) This identity reduces to

$$2 \int \mathrm{d}\hat{U} \left[\begin{pmatrix} U \\ \mathbf{1} \end{pmatrix}^* \mathcal{C}\mathcal{T}^E(N,0)^* \mathcal{T}^E(N,0)\mathcal{C}^* \begin{pmatrix} U \\ \mathbf{1} \end{pmatrix} \right]^{-1} = \mathbf{1}.$$

Now $\mathcal{T}^E(N,0)^*\mathcal{T}^E(N,0)$ is a positive symplectic matrix and hence $\mathcal{C}\mathcal{T}^E(N,0)^*\mathcal{T}^E(N,0)\mathcal{C}^*$ is a positive matrix in $\mathrm{U}(L,L)$. Hence lemma 1 shows that this identity indeed holds.

□

4. Spectral measures averaged over coupling constants

As an application of the results of theorem 3 we consider here a particular one-parameter family of Jacobi matrices with matrix entries obtained by a local positive perturbation and show that the associated averaged spectral measure is under certain conditions absolutely continuous.

Let H be a Jacobi matrix with matrix entries in the limit point case, and let $\pi_n : \mathbb{C}^L \to (\mathbb{C}^L)^{\mathbb{N}}$ denote the partial isometry onto the nth site. For real positive semi-definite matrices $(W_n)_{1\leqslant n\leqslant N}$ and $\mu \in \mathbb{R}$ define

$$H(\mu) = H + \mu \sum_{n=1}^{N} \pi_n W_n \pi_n^*.$$

Furthermore, let $H^N(\mu)$ be the finite Jacobi matrix obtained by projecting $H(\mu)$ to the first N sites. It is of the form (3) with V_n replaced by $V_n + \mu W_n$ and $\hat{Z} = Z = 0$. Because the perturbation $H(\mu) - H$ is increasing in μ, the eigenvalues of $H(\mu)$ are increasing functions of μ. Finally let $\rho(\mu)$ be the matrix-valued spectral measure of $H(\mu)$ and define the averaged spectral measure corresponding to an interval $I = [\mu_0, \mu_1]$ by

$$\overline{\rho} = \int_I \mathrm{d}\mu \mathrm{Tr}(\rho(\mu)).$$

Theorem 5. *Suppose that $W_n > 0$ and $W_{n+1} > 0$ for some $n = 1, \ldots, N-1$. Let $I = [\mu_0, \mu_1]$ be sufficiently large such that there are $2L$ eigenvalues of $H^N(\mu)$ passing by E as μ varies in I. Then $\overline{\rho}$ is equivalent to the Lebesgue measure in a neighborhood of E.*

As can be seen from the proof below the hypothesis can be somewhat relaxed. For $L = 1$ the result was proven in [dRMS]. Similar as in [dRMS], the condition on the size of I can also expressed in terms of an associated Birman–Schwinger operator and, furthermore, it is also possible to consider several parameter spectral averaging instead of over just one parameter μ. On the other hand, the applications to spectral analysis do not carry over immediately, because the subordinacy theory is not yet developed for Jacobi matrices with matrix entries.

First we need to fix some notations. Just as $H(\mu)$, all objects of the previous sections depend on a supplementary parameter μ. In particular, we will write $\mathcal{T}^z_n(\mu)$ and $\mathcal{T}^z(n, m, \mu)$. Furthermore, let us introduce the Dirichlet solutions $\Psi^{\mathrm{D},z}_N(\mu) = \mathcal{T}^z(N, 0, \mu)\binom{\mathbf{1}}{0}$ and the matrix

$$P^E_N(\mu) = -\Psi^{\mathrm{D},E}_N(\mu)^*\mathcal{J}\partial_\mu\Psi^{\mathrm{D},E}_N(\mu).$$

The proof of theorem 5 will be based on the following criterion.

Lemma 2. *Suppose (i) There exist positive constants C_1, C_2 such that $C_1\mathbf{1} \leqslant P^E_N(\mu) \leqslant C_2\mathbf{1}$ for all $\mu \in I$. (ii)*

$$\int_I \frac{\mathrm{d}\mu}{2\pi}\,\mathrm{Im}m\,\partial_\mu \log\big(\Pi(\Psi^{\mathrm{D},E}_N(\mu))\big) < -L.$$

Then $\overline{\rho}$ is equivalent to the Lebesgue measure in a neighborhood of E.

Proof. We write $\overline{\rho}(E_0, E_1)$ for $\frac{1}{2}\big[\overline{\rho}([E_0, E_1]) + \overline{\rho}((E_0, E_1))\big]$. Let us start by integrating (19) over μ and using the dominated convergence theorem as well as Fubini's theorem:

$$\overline{\rho}(E_0, E_1) = \lim_{M\to\infty}\int_{E_0}^{E_1}\mathrm{d}E\int_I \mathrm{d}\mu\,\mathrm{Tr}\big(\big|\mathcal{T}^E(M, N)\Psi^{\mathrm{D},E}_N(\mu)\big|^{-2}\big).$$

Now for positive semi-definite operators A, B with $0 < C_1\mathbf{1} \leqslant B \leqslant C_2\mathbf{1}$,

$$\frac{1}{C_2}\mathrm{Tr}(AB) \leqslant \mathrm{Tr}(A) \leqslant \frac{1}{C_1}\mathrm{Tr}(AB).$$

Applying these bounds for $B = P^E_N(\mu)$ shows that

$$\overline{\rho}(E_0, E_1) \approx \lim_{M\to\infty}\int_{E_0}^{E_1}\mathrm{d}E\int_I \mathrm{d}\mu\,\mathrm{Tr}\big(\big|\mathcal{T}^E(M, N)\Psi^{\mathrm{D},E}_N(\mu)\big|^{-2}P^E_N(\mu)\big),$$

where the sign $\approx$ means that we have two-sided bounds. As $\mathcal{T}^E(M, N)^*\mathcal{J}\mathcal{T}^E(M, N) = \mathcal{J}$, $\Psi^{\mathrm{D},E}_M(\mu) = \mathcal{T}^E(M, N)\Psi^{\mathrm{D},E}_N(\mu)$ and $\mathcal{T}^E(M, N)$ does not depend on μ, this can be rewritten as

$$\begin{aligned}\overline{\rho}(E_0, E_1) &\approx -\lim_{M\to\infty}\int_{E_0}^{E_1}\mathrm{d}E\int_I \mathrm{d}\mu\,\mathrm{Tr}\big(\big|\Psi^{\mathrm{D},E}_M(\mu)\big|^{-2}\Psi^{\mathrm{D},E}_M(\mu)^*\mathcal{J}\partial_\mu\Psi^{\mathrm{D},E}_M(\mu)\big)\\ &= -\pi\lim_{M\to\infty}\int_{E_0}^{E_1}\mathrm{d}E\int_I\frac{\mathrm{d}\mu}{2\pi}\,\mathrm{Im}m\,\partial_\mu\log\big(\Pi(\Psi^{\mathrm{D},E}_M(\mu))\big),\end{aligned}$$

where the second identity is checked in [SB1][lemma 4]. Now the expression under the integral $\int \mathrm{d}E$ on the rhs is precisely the pairing $\int_\Gamma \omega$ of the Arnold cocycle ω with the path $\Gamma(\mu) = \Psi^{\mathrm{D},E}_M(\mu) = \mathcal{T}^E(M, N)\Psi^{\mathrm{D},E}_N(\mu)$, $\mu \in I$, in the Lagrangian Grassmannian $\mathbb{L}_L$ (actually here this is a path in the real Lagrangian Grassmannian because $H(\mu)$ is real). Hypothesis states something about the pairing with the path $\Gamma'(\mu) = \Psi^{\mathrm{D},E}_N(\mu)$, namely $\int_{\Gamma'}\omega < -L$. However, these two paths are related by the multiplication with the symplectic matrix $\mathcal{T}^E(M, N)$. Hence by [SB1], [proposition 4]

$$\left|\int_\Gamma \omega - \int_{\Gamma'}\omega\right| \leqslant L.$$

Therefore $0 < C_3 < -\displaystyle\int_\Gamma \omega < C_4$ where the upper bound follows from compactness of I and the constants are independent of M. Replacing this shows

$$\overline{\rho}(E_0, E_1) \approx \lim_{M\to\infty}\int_{E_0}^{E_1}\mathrm{d}E = E_1 - E_0,$$

which is precisely the claimed equivalence of $\overline{\rho}$ with the Lebesgue measure.

□

Proof of theorem 5. First of all,

$$\mathcal{T}^E(N,0,\mu)^*\mathcal{J}^*\partial_\mu\mathcal{T}^E(N,0,\mu) = \sum_{n=1}^{N}\mathcal{T}^E(n-1,0,\mu)^*\mathcal{T}_n^E(\mu)^*\mathcal{J}^*(\partial_\mu\mathcal{T}_n^E(\mu))\,\mathcal{T}^E(n-1,0,\mu).$$

But

$$\mathcal{T}_n^E(\mu)^*\mathcal{J}^*\partial_\mu\mathcal{T}_n^E(\mu) = \begin{pmatrix}\left(T_n^{-1}\right)^* W_n T_n^{-1} & 0\\ 0 & 0\end{pmatrix}$$

is positive semi-definite, and the arguments in the proof of [SB1][proposition 6] show that

$$\begin{pmatrix}\left(T_{n+1}^{-1}\right)^* W_{n+1} T_{n+1}^{-1} & 0\\ 0 & 0\end{pmatrix} + \mathcal{T}_{n+1}^E(\mu)^*\begin{pmatrix}\left(T_n^{-1}\right)^* W_n T_n^{-1} & 0\\ 0 & 0\end{pmatrix}\mathcal{T}_{n+1}^E(\mu) > 0$$

(strict positivity), whenever $W_n > 0$ and $W_{n+1} > 0$. In the latter case the above sum is therefore strictly positive. Hence the hypothesis of theorem 5 implies $P_N^E(\mu) \geqslant C_1 > 0$. Compactness of I thus implies that hypothesis (i) of lemma 2 holds. Hypothesis (ii) follows from the oscillation theorem as stated in theorem 1. In fact, as μ increases each phase $\theta_{N,l}^E(\mu)$ decreases. The integral in (ii) is the total phase (sum of all $\theta_{N,l}^E(\mu)$'s, in units of 2π) accumulated as μ varies in I. If $L + K$ eigenvalues pass by E as μ varies, the total phase has to change by at least K. Hence the hypothesis of theorem 5 imply (ii) of lemma 2.

□

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Appendix A. Reminder on Möbius transformations

This appendix resembles the basic properties of the Möbius transformation as they are used in the main text. All proofs are contained in [SB1]. Complex matrices of size $2L \times 2L$ are denoted by mathcal symbols, those of size $L \times L$ by roman letters.

The upper half-plane and unit disc (also called Cartan's first classical domain) are defined by

$$\mathbb{U}_L = \left\{Z \in \mathrm{Mat}(L\times L,\mathbb{C})\,\middle|\,\imath(Z^*-Z)>0\right\}, \qquad \mathbb{D}_L = \left\{U \in \mathrm{Mat}(L\times L,\mathbb{C})\,\middle|\,U^*U<\mathbf{1}\right\},$$

where $Y > 0$ means that Y is positive definite. If $Z \in \mathbb{U}_L$, then Z is invertible and $-Z^{-1} \in \mathbb{U}_L$. Moreover, for any $V = V^*$ and any invertible T, one has $Z + V \in \mathbb{U}_L$ and $T^*ZT \in \mathbb{U}_L$. The formulae

$$U = (Z-\imath\mathbf{1})(Z+\imath\mathbf{1})^{-1}, \qquad Z = \imath(\mathbf{1}+U)(\mathbf{1}-U)^{-1}, \tag{A.1}$$

establish an analytic diffeomorphism from $\mathbb{U}_L$ onto $\mathbb{D}_L$. The boundary $\partial\mathbb{D}_L$ of $\mathbb{D}_L$ is a stratified space given as the union of strata $\partial_l\mathbb{D}_L, l = 1,\ldots,L$, where $\partial_l\mathbb{D}_L$ is the set of matrices U for which $U^*U \leqslant \mathbf{1}$ and rank $(\mathbf{1}-U^*U) = L-l$. By proposition 2 the maximal boundary $\partial_L\mathbb{D}_L = \mathrm{U}(L)$ is identified with the Lagrangian Grassmannian $\mathbb{L}_L$. Similarly, the boundary of $\mathbb{U}_L$ is stratified, but this will play no role here.

The Möbius transformation (also called canonical transformation or fractional transformation) is defined by

$$\mathcal{T}\cdot Z = (AZ+B)(CZ+D)^{-1},$$
$$\mathcal{T} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in \mathrm{GL}(2L,\mathbb{C}), \qquad Z \in \mathrm{Mat}(L\times L,\mathbb{C}), \tag{A.2}$$

whenever the appearing inverse exists. For $\mathcal{T}$ as in (A.2) and as long as the appearing inverse exists, the inverse Möbius transformation is defined by

$$W : \mathcal{T} = (WC-A)^{-1}(B-WD), \qquad W \in \mathrm{Mat}(L\times L,\mathbb{C}). \tag{A.3}$$

The Möbius transformation is a left action, namely $(\mathcal{T}\mathcal{T}')\cdot Z = \mathcal{T}\cdot(\mathcal{T}'\cdot Z)$ as long as all objects are well defined. It is well known that if $\mathcal{T}\in \mathrm{SP}\,(2L,\mathbb{C})$ and $Z\in\mathbb{U}_L$, the Möbius transformation $\mathcal{T}\cdot Z$ is well defined.

Appendix B. Cauchy formula for Cartan's classical domain

The results of this section are proven in [Hua]. Let $\overline{\mathbb{D}_L}$ be the topological closure of $\mathbb{D}_L$ and let $\mathrm{d}U$ be the normalized Haar measure on its maximal boundary $\partial_L\mathbb{D}_L = \mathrm{U}(L)$.

Theorem 6. *For any continuous function $f:\overline{\mathbb{D}_L}\to\mathbb{C}$ which is analytic on $\mathbb{D}_L$, one has for all $Z\in\mathbb{D}_L$,*

$$f(Z) = \int \mathrm{d}U\,\det(\mathbf{1}-ZU^*)^{-L} f(U). \tag{B.1}$$

For the proof of theorem 2 we only need the case $Z=\mathbf{0}$. Moreover, only intervene functions f which are of the form $f(U)=F(\mathcal{C}^*\cdot U)$ where $\mathcal{C}^*\cdot U$ is the Cayley transform of a unitary matrix (written in the notations of the appendix) and hence Hermitian, and F is a complex function on the Hermitian matrices. The Cayley transform $\mathcal{C}^*\cdot U$ is not defined for all unitaries U, but it is defined on a set of full measure. The change of variables formula to the Lebesgue measure $\mathrm{d}\xi$ on (real and imaginary parts of each entry of) the Hermitian matrices is now

$$\int \mathrm{d}U\,F(\mathcal{C}^*\cdot U) = c\int \mathrm{d}\xi\,\det(\mathbf{1}+\xi^*\xi)^{-L}F(\xi),$$

where c is a normalization constant (which is given in [Hua]). As the measure $\mathrm{d}\xi\,\det(\mathbf{1}+\xi^*\xi)^{-L}$ is invariant under the reflection $\xi\mapsto-\xi$, it follows that

$$\int \mathrm{d}U\,F(\mathcal{C}^*\cdot U) = \int \mathrm{d}U\,F(-\mathcal{C}^*\cdot U). \tag{B.2}$$

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