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Rotation numbers for Jacobi matrices with matrix entries

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Abstract

A Jacobi matrix with matrix entries is a selfadjoint block tridiagonal matrix with positive definite blocks on the off-diagonals. A rotation number calculation for its eigenvalues is presented. This is a matricial generalization of the oscillation theorem for the discrete analogues of Sturm-Liouville operators. The three universality classes of time reversal invariance are dealt with by implementing the corresponding symmetries. For Jacobi matrices with random matrix entries, this leads to a formula for the integrated density of states which can be calculated perturbatively in the coupling constant of the randomness with an optimal control on the error terms.

1 Introduction

This article is about matrices of the type

$$H^N = \begin{pmatrix} V_1 & T_2 & & & & \\ T_2 & V_2 & T_3 & & & \\ & T_3 & V_3 & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & V_{N-1} & T_N \\ & & & & T_N & V_N \end{pmatrix}, \qquad (1)$$

where $V_n = V_n^*$ are selfadjoint complex $L \times L$ matrices and T_n are positive definite complex $L \times L$ matrices. With the convention $T_1 = \mathbf{1}$ and for a complex energy $E \in \mathbb{C}$, introduce the transfer matrices

$$\mathcal{T}_n^E \;=\; \begin{pmatrix} (E\,\mathbf{1} - V_n)\,T_n^{-1} & -T_n \\ T_n^{-1} & \mathbf{0} \end{pmatrix}\,, \qquad n = 1, \ldots, N\,. \tag{2}$$

Then set

$$U_N^E \;=\; \begin{pmatrix} \mathbf{1} \\ \imath\,\mathbf{1} \end{pmatrix}^* \prod_{n=1}^{N} \mathcal{T}_n^E \begin{pmatrix} \mathbf{1} \\ \mathbf{0} \end{pmatrix} \left(\begin{pmatrix} \mathbf{1} \\ \imath\,\mathbf{1} \end{pmatrix}^t \prod_{n=1}^{N} \mathcal{T}_n^E \begin{pmatrix} \mathbf{1} \\ \mathbf{0} \end{pmatrix} \right)^{-1}\,. \tag{3}$$

Theorem 1 *Let $E \in \mathbb{R}$ and $N \geq 2$.*
(i) *U_N^E is well-defined, namely the appearing inverse exists.*
(ii) *U_N^E is a unitary matrix which is real analytic in E.*
(iii) *The real eigenphases $\theta_{N,l}^E$, $l = 1, \ldots, L$, of U_N^E can be chosen (at level crossings) to be analytic in E and such that $\theta_{N,l}^E \to 0$ as $E \to -\infty$ and $\theta_{N,l}^E \to 2\pi N$ as $E \to \infty$.*
(iv) *E is an eigenvalue of H^N of multiplicity m if and only if $\theta_{N,l}^E = \pi \bmod 2\pi$ for exactly m of the indices $l = 1, \ldots, L$.*
(v) *The matrix $S_N^E = \frac{1}{\imath}\,(U_N^E)^* \partial_E U_N^E$ is positive definite. Each $\theta_{N,l}^E$ is an increasing function of E.*
(vi) *If H^N is real, the unitary U_N^E is symmetric and the positive matrix S_N^E is real.*
(vii) *Let L be even and let*

$$I \;=\; \begin{pmatrix} \mathbf{0} & -\mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix} \;\in\; \mathrm{Mat}(L \times L, \mathbb{C}) \tag{4}$$

with 4 blocks of size $\frac{L}{2} \times \frac{L}{2}$. Suppose that H^N is self-dual, namely the entries are self-dual:

$$I^*\,T_n^t\,I \;=\; T_n\,, \qquad I^*\,V_n^t\,I \;=\; V_n\,, \qquad n = 1, \ldots, N\,.$$

Then U_N^E and S_N^E are also self-dual (equivalently, IU_N^E and IS_N^E are skew-symmetric).

Items (i), (ii), (iv), (vi) and (vii) result directly from the mathematical set-up, while the analyticity statements of items (ii) and (iii) are based on elementary analytic perturbation theory [Kat]. The second part of (iii) follows from a homotopy argument and item (v), even though a consequence of a straight-forward calculation, is the main mathematical insight. It justifies the term *rotation numbers* for the eigenphases. In the strictly one-dimensional situation and for Sturm-Liouville operators instead of Jacobi matrices, the theorem has been known for almost two centuries as the rotation number calculation or the Sturm-Liouville oscillation theorem [Wei, JM]. For matricial Sturm-Liouville operators, Bott [Bot] has proven results related to the above theorem. (The author learned of Bott's work once this article was finished, and believes that the techniques presented below allow to considerably simplify Bott's proof. A detailed treatment is under preparation.) For related work on linear Hamiltonian system let us refer to the review [FJN]. The discrete one-dimensional case and hence precisely the case $L = 1$ of Theorem 1 is also well-known (see *e.g.* [JSS] for a short proof). A rougher result was proven by Arnold [Arn2]. In the one-dimensional situation the variable $\theta^E_{N,1}$ is called the Prüfer phase. Therefore one may refer to the eigenphases $\theta^E_{N,l}$ (or the unitaries U^E_N themselves) also as multi-dimensional Prüfer phases. The two supplementary symmetries considered in items (vi) and (vii) correspond to quantum-mechanical Hamiltonians H^N with time-reversal invariance describing systems with odd or even spin respectively [Meh]. This notion is empty in the one-dimensional situation where time-reversal invariance follows automatically from self-adjointness.

Crucial ingredient of the proof is that (3) for real energies actually stems from the Möbius action of the symplectic transfer matrices (2) on the unitary matrices (Theorem 5), which in turn are diffeomorphic to the Lagrangian Grassmannian via the stereographic projection (Theorem 4). As a function of real energy, U^E_N hence corresponds to a path of Lagrangian planes. If one defines a singular cycle in the unitary group as the set of unitaries with eigenvalue -1, then the intersections of the above path with this cycle turn out to be precisely at the eigenvalues of H^N.

One new perspective opened by Theorem 1 concerns Jacobi matrices with random matrix entries, describing *e.g.* finite volume approximations of the higher-dimensional Anderson model. In fact, the unitary, symmetric unitary and anti-symmetric unitary matrices form precisely the state spaces of Dyson's circular ensembles. They are furnished with unique invariant measures (Haar measures on the corresponding symmetric spaces). A good working hypothesis is hence that the random dynamical system induced by the action of the symplectic transfer matrices on the unitary matrices has an invariant measure (in the sense of Furstenberg [BL]) which is invariant under the unitary group. This can only be true to lowest order in perturbation theory, under a hypothesis on the coupling of the randomness (which has to be checked for concrete models), and on a set of lower dimensional unitary matrices corresponding to the elliptic channels (in the sense of [SB] and Section 4). This unitary invariance on the elliptic channels would justify the random phase approximation or maximal entropy Ansatz (here as equidistribution of Lagrangian planes) widely used in the physics community in the study of quasi-one-dimensional systems to establish a link between random models like the Anderson Hamiltonian and invariant random matrix ensembles (*e.g.* [Bee]). Furthermore, let us consider H^N describing a physical system on a d-dimensional cube, namely with $L = N^{d-1}$, and suppose d sufficiently large. Then a further working hypothesis is that the positive matrices $\frac{1}{N}S^E_N$ are distributed according to the Wishard ensemble of adequate symmetry (again on the elliptic subspaces and in the weak coupling limit). If both working hypothesis turn out to hold and U^E_N and S^E_N are asymptotically independent, namely randomly rotated w.r.t. each other (for large cubes), then Theorem 1 combined with a convolution argument shows that the level statistics of H^N is asymptotically given by the

Wigner-Dyson statistics for quantum systems without or with time-reversal invariance for odd or even spin, according to the symmetry of H^N. Roughly, Theorem 1 hence gives one possible way to make the heuristics given in the introduction to Chapter 9 of Mehta's book [Meh] more precise. Numerics supporting the above have been carried out in collaboration with R. Römer.

As a first application of Theorem 1 and the techniques elaborated in its proof we develop in Section 4 the lowest order perturbation theory for the integrated density of states (IDS) of a semi-infinite real Jacobi matrix with random matrix entries. More precisely, we suppose that the entries in (1) are of the form $V_n = V(\mathbf{1} + \lambda\, v_n + \mathcal{O}(\lambda^2))$ and $T_n = T(\mathbf{1} + \lambda\, t_n + \mathcal{O}(\lambda^2))$ where V, T, v_n, t_n are real symmetric matrices and T is positive definite. The v_n, t_n are drawn independently and identically from a bounded ensemble $(v_\sigma, t_\sigma)_{\sigma\in\Sigma}$ according to a given distribution $\mathbf{E}_\sigma$, and furthermore the dependence on the coupling constant $\lambda \geq 0$ is real analytic and the error terms satisfy norm estimates. Associated to a random sequence $\omega = (v_n, t_n)_{n\geq 1}$ are random real Hamiltonians $H^N(\omega, \lambda)$. The Anderson model on a strip is an example within this class of models. The number of eigenvalues of $H^N(\omega, \lambda)$ smaller than a given energy E and per volume element NL is a self-averaging quantity in the limit $N \to \infty$ which converges to the IDS $\mathcal{N}_\lambda(E)$ (see Section 4 for the formal definition). Let furthermore $\mathcal{N}_{\lambda,\sigma}(E)$ denote the IDS of the translation invariant Hamiltonian with $\omega = (v_\sigma, t_\sigma)_{n\geq 1}$. Finally let $\mathcal{T}^E$ be the transfer matrix defined as in (2) from the unperturbed entries V and T.

Theorem 2 *Suppose that $E \in \mathbb{R}$ is such that $\mathcal{T}^E$ is diagonalizable and does not have anomalies, namely the rotation phases of the elliptic channels are incommensurate* (*cf.* Section 4.2 *for the precise hypothesis*). *Then*

$$\mathcal{N}_\lambda(E) \;=\; \mathbf{E}_\sigma\big(\mathcal{N}_{\lambda,\sigma}(E)\big) \;+\; \mathcal{O}(\lambda^2)\;. \tag{5}$$

The same result holds for random perturbations of arbitrary periodic operators. The fact that $\mathcal{T}^E$ is not allowed to have any Jordan blocks means that E is not an internal band edge. Together with the anomalies they form a discrete set of excluded energies. The main point of Theorem 2 is not the calculation of the leading order term in λ (which is indeed given by the most naive guess), but rather the control of the error term which is uniform in L as long as one stays uniformly bounded away from anomalies and internal band edges. The estimates in Section 4.2 also show how the error bound diverges as one approaches these energies. However, this part of the analysis is not optimized and there is a definite need for refinement in order to be able to study the thermodynamic limit of solid state physics models. The error bound is nevertheless optimal in the sense that the $\mathcal{O}(\lambda^2)$ contribution on the l.h.s. does depend on further details of the model. Similar as in the one-dimensional situation ($L = 1$), the IDS and the sum of the positive Lyapunov exponents are imaginary and real boundary values of a single Herglotz function [KS]. Hence we also develop a perturbation theory for the sum of the Lyapunov exponents, with a considerably better control on the error terms than in [SB] where a particular case has been treated.

This work is organized as follows. The next section recollects the tools from symplectic geometry used in the proof of Theorem 1. In particular, it is shown that the Möbius action of the symplectic group on the unitary matrices is well-defined and furthermore some formulas for the calculation of the intersection number (Maslov index) are given. Section 3 provides the proof of Theorem 1 and then gives some supplementary results on Jacobi matrices with matrix entries and their spectra. Section 4 contains the definition of the IDS for Jacobi matrices with random matrix entries and a formula for the associated averaged Lyapunov exponent. Then the proof of Theorem 2 is given.

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2 Symplectic artillery

Apart from the propositions in Section 2.8 which may be strictly speaking new, this section is probably known to the experts in symplectic geometry. But there does not seem to be reference with a treatment as compact and unified as the present one. The author's references were [Hua, Sie, Arn1, CL, KoS, Arn3] and he hereby excuses for not citing all the interesting works that he does not know of. The reader is warned that the complex Lagrangian planes and the complex symplectic group are defined with the adjoint rather than the transpose. This differs from standard references, but hopefully the reader will agree that it is natural in the present context.

Let us introduce some notations. The following $2L \times 2L$ matrices (matrices of this size are denoted by mathcal symbols in this work) are composed by 4 blocks of size $L \times L$:

$$\mathcal{J} = \begin{pmatrix} \mathbf{0} & -\mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix}, \quad \mathcal{G} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}, \quad \mathcal{C} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1} & -\imath\mathbf{1} \\ \mathbf{1} & \imath\mathbf{1} \end{pmatrix}, \quad \mathcal{I} = \begin{pmatrix} \mathbf{0} & -I \\ I & \mathbf{0} \end{pmatrix},$$

where in the last equation I is given by (4) and hence L is supposed to be even. $\mathcal{J}$ is called the symplectic form, $\mathcal{C}$ the Cayley transform and $\mathcal{I}$ the self-duality transform. The following identities will be useful:

$$\mathcal{C}\,\mathcal{J}\,\mathcal{C}^* = \frac{1}{\imath}\,\mathcal{G}\,, \qquad \overline{\mathcal{C}}\,\mathcal{J}\,\mathcal{C}^* = \frac{1}{\imath}\,\mathcal{J}\,, \qquad \overline{\mathcal{C}}\,\mathcal{I}\,\mathcal{C}^* = \frac{1}{\imath}\,\mathcal{I}\,. \tag{6}$$

In order to deal with the symmetry of Theorem 1(vii), hence L even, some further notations are convenient. A matrix $A \in \mathrm{Mat}(L \times L, \mathbb{C})$ is call self-dual if $I^* A^t I = A$, and it is called self-conjugate if $I^*\overline{A}I = A$. As already indicated in Theorem 1(vii), self-duality is closely linked to skew-symmetry, namely A is self-dual if and only if $(IA)^t = -IA$. The sets of skew-symmetric and self-dual matrices are denoted by $\mathrm{Skew}(L,\mathbb{C})$ and $\mathrm{Self}(L,\mathbb{C})$ respectively. Moreover, for selfadjoint matrices $A^* = A$ the notions of self-duality and self-conjugacy coincide.

2.1 Lagrangian Grassmannian

The set of L-dimensional subspaces of the complex vector space $\mathbb{C}^{2L}$ is denoted by $\mathbb{G}_L^{\mathbb{C}}$. The vectors of a basis of such a plane form the column vectors of a $2L \times L$ matrix Φ which has rank L. Of course, a plane does not depend on the choice of the basis (and hence the explicit form of Φ). Consider the relation: $\Phi \sim \Psi \Leftrightarrow$ there exists $c \in \mathrm{Gl}(L,\mathbb{C})$ with $\Phi = \Psi c$. The Grassmannian $\mathbb{G}_L^{\mathbb{C}}$ is then the set of equivalence classes w.r.t. $\sim$:

$$\mathbb{G}_L^{\mathbb{C}} \;=\; \{[\Phi]_\sim \mid \Phi \in \mathrm{Mat}(2L\times L,\mathbb{C})\;,\;\; \mathrm{rank}(\Phi) = L\;\}\;.$$

A plane is called (complex hermitian) Lagrangian if $\Phi^*\mathcal{J}\Phi = \mathbf{0}$. Here $A^* = \overline{A}^t$ denotes transpose of the complex conjugate of a matrix A. If $\Phi = \begin{pmatrix} a \\ b \end{pmatrix}$ where a and b are complex $L\times L$ matrices, the latter condition means that $a^*b = b^*a$ is selfadjoint. The (complex hermitian) Lagrangian Grassmannian $\mathbb{L}_L^{\mathbb{C}}$ is the set of Lagrangian planes:

$$\mathbb{L}_L^{\mathbb{C}} \;=\; \{[\Phi]_\sim \mid \Phi \in \mathrm{Mat}(2L\times L,\mathbb{C})\;,\;\; \mathrm{rank}(\Phi) = L\;,\;\; \Phi^*\mathcal{J}\Phi = \mathbf{0}\;\}\;. \tag{7}$$

This is a real analytic manifold. It contains the submanifold $\mathbb{L}_L^{\mathbb{R}}$ of real Lagrangian planes:

$$\mathbb{L}_L^{\mathbb{R}} \;=\; \left\{[\Phi]_\sim \;\middle|\; \Phi \in \mathrm{Mat}(2L\times L,\mathbb{C})\;,\;\; \mathrm{rank}(\Phi) = L\;,\;\; \Phi^*\mathcal{J}\Phi = \mathbf{0}\;,\;\; \Phi^t\mathcal{J}\Phi = \mathbf{0}\;\right\}\;. \tag{8}$$

Hence $\mathbb{L}_L^{\mathbb{R}}$ is a subset of $\mathbb{L}_L^{\mathbb{C}}$ characterized by a supplementary symmetry. That this coincides with the usual definition of the real Lagrangian Grassmannian is stated in Theorem 3 below. If L is even, then $\mathbb{L}_L^{\mathbb{C}}$ contains another submanifold characterized by another symmetry:

$$\mathbb{L}_L^{\mathbb{H}} \;=\; \left\{[\Phi]_\sim \;\middle|\; \Phi \in \mathrm{Mat}(2L\times L,\mathbb{C})\;,\;\; \mathrm{rank}(\Phi) = L\;,\;\; \Phi^*\mathcal{J}\Phi = \mathbf{0}\;,\;\; \Phi^t\mathcal{I}\Phi = \mathbf{0}\;\right\}\;. \tag{9}$$

The notation $\mathbb{L}_L^{\mathbb{H}}$ appealing to the quaternions is justified by the following theorem, in which $\mathbb{H}^L$ is considered as a vector space over $\mathbb{C}$. Let $A^{*_{\mathbb{H}}}$ denote the transpose and quaternion conjugate (inversion of sign of all three imaginary parts) of a matrix A with quaternion entries. Similarly, $A^{*_{\mathbb{R}}} = A^t$ for a matrix with real entries.

Theorem 3 *One has, with equality in the sense of diffeomorphic real analytic manifolds,*

$$\mathbb{L}_L^{\mathbb{R}} \;=\; \{[\Phi]_\sim \mid \Phi \in \mathrm{Mat}(2L\times L,\mathbb{R})\;,\;\; \mathrm{rank}(\Phi) = L\;,\;\; \Phi^{*_{\mathbb{R}}}\mathcal{J}\Phi = \mathbf{0}\;\}\;,$$

and

$$\mathbb{L}_L^{\mathbb{H}} \;=\; \{[\Phi]_\sim \mid \Phi \in \mathrm{Mat}(L\times L,\mathbb{H})\;,\;\; \mathrm{rank}(\Phi) = L\;,\;\; \Phi^{*_{\mathbb{H}}}I\Phi = \mathbf{0}\;\}\;.$$

The proof is postponed to the next section.

2.2 Stereographic projection

Bott [Bot] showed that the complex Lagrangian Grassmannian $\mathbb{L}_L^{\mathbb{C}}$ is homeomorphic to the unitary group $\mathrm{U}(L)$, a fact that was rediscovered in [KoS, Arn3]. Arnold [Arn1] used the fact that $\mathbb{L}_L^{\mathbb{R}}$ can be identified with $\mathrm{U}(L)/\,\mathrm{O}(L)$. Indeed, a real Lagrangian plane can always be spanned by an orthonormal system, that is, be represented by Φ satisfying $\Phi^*\Phi = \mathbf{1}$. This induces $(\Phi, \mathcal{J}\Phi) \in \mathrm{SP}(2L, \mathbb{R}) \cap \mathrm{O}(2L) \cong \mathrm{U}(L)$. Of course, various orthonormal systems obtained by orthogonal basis changes within the plane span the same Lagrangian plane. Hence $\mathbb{L}_L^{\mathbb{R}} \cong \mathrm{U}(L)/\,\mathrm{O}(L)$. Moreover, the symmetric space $\mathrm{U}(L)/\,\mathrm{O}(L)$ can be identified with the unitary symmetric matrices by sending a right equivalence class $A\,\mathrm{O}(L) \in \mathrm{U}(L)/\,\mathrm{O}(L)$ to AA^t. As these facts will be crucial later on, let us give a detailed proof and some explicit formulas.

The stereographic projection π is defined on the subset

$$\mathbb{G}_L^{\mathrm{inv}} \;=\; \left\{ [\Phi]_\sim \in \mathbb{G}_L \;\middle|\; \begin{pmatrix} \mathbf{0} & \mathbf{1} \end{pmatrix} \Phi \;\in\; \mathrm{GL}(L, \mathbb{C}) \right\} \;,$$

by

$$\pi([\Phi]_\sim) \;=\; \begin{pmatrix} \mathbf{1} & \mathbf{0} \end{pmatrix} \Phi \left(\begin{pmatrix} \mathbf{0} & \mathbf{1} \end{pmatrix} \Phi \right)^{-1} \;=\; a\, b^{-1} \;, \qquad \Phi \;=\; \begin{pmatrix} a \\ b \end{pmatrix} \;.$$

One readily checks that $\pi([\Phi]_\sim)$ is independent of the representative. If $[\Phi]_\sim \in \mathbb{L}_L^{\mathbb{C}} \cap \mathbb{G}_L^{\mathrm{inv}}$, then $\pi([\Phi]_\sim)$ is selfadjoint. The fact that π is not defined on all of $\mathbb{L}_L^{\mathbb{C}}$ is an unpleasant feature that can be circumvented by use of Π defined by

$$\Pi([\Phi]_\sim) \;=\; \pi([\mathcal{C}\,\Phi]_\sim) \;, \qquad \text{if } \; [\mathcal{C}\,\Phi]_\sim \in \mathbb{G}_L^{\mathrm{inv}} \;.$$

Theorem 4 (i) *The map* $\Pi : \mathbb{L}_L^{\mathbb{C}} \to \mathrm{U}(L)$ *is a real analytic diffeomorphism.*
(ii) *The map* $\Pi : \mathbb{L}_L^{\mathbb{R}} \to \mathrm{U}(L) \cap \mathrm{Sym}(L, \mathbb{C})$ *is a real analytic diffeomorphism.*
(iii) *Let* L *be even. The map* $\Pi : \mathbb{L}_L^{\mathbb{H}} \to \mathrm{U}(L) \cap \mathrm{Self}(L, \mathbb{C})$ *is a real analytic diffeomorphism.*

Proof. Let $\Phi = \begin{pmatrix} a \\ b \end{pmatrix}$ where a and b are $L \times L$ matrices satisfying $a^* b = b^* a$. One has

$$\begin{aligned} L \;&=\; \mathrm{rank}(\Phi) \;=\; \mathrm{rank}(\Phi^*\Phi) \;=\; \mathrm{rank}(a^*a + b^*b) \\ &=\; \mathrm{rank}\big((a + \imath\, b)^*(a + \imath\, b)\big) \;=\; \mathrm{rank}(a + \imath\, b) \;=\; \mathrm{rank}(a - \imath\, b) \;. \end{aligned} \tag{10}$$

It follows that $[\mathcal{C}\Phi]_\sim \in \mathbb{G}_L^{\rm inv}$ so that it is in the domain of the stereographic projection π and hence Π is well-defined. Next let us show that the image is unitary. It follows from (10) and a short calculation (or alternatively the first identity in (6)) that

$$\mathcal{C}\,\mathbb{L}_L^{\mathbb{C}} \;=\; \left\{ \left[\begin{pmatrix} a \\ b \end{pmatrix}\right]_\sim \;\middle|\; a,b\in \mathrm{GL}(L,\mathbb{C})\;,\;\; a^*a=b^*b \right\}\;.$$

Hence if $[\mathcal{C}\Phi]_\sim = \left[\begin{pmatrix} a \\ b \end{pmatrix}\right]_\sim \in \mathcal{C}\,\mathbb{L}_L^{\mathbb{C}}$, one has

$$\Pi([\Phi]_\sim)^*\Pi([\Phi]_\sim) \;=\; (b^*)^{-1}a^*a\,b^{-1} \;=\; \mathbf{1}\;.$$

Moreover, Π is continuous. One can directly check that the inverse of Π is given by

$$\Pi^{-1}(U) \;=\; \left[\begin{pmatrix} \frac{1}{2}(U+\mathbf{1}) \\ \frac{\imath}{2}(U-\mathbf{1}) \end{pmatrix}\right]_\sim\;. \tag{11}$$

As this is moreover real analytic, this proves (i).

For the case (ii) of the real Lagrangian Grassmannian, the second identity of (6) implies that the supplementary symmetry in (8) leads to

$$\mathcal{C}\,\mathbb{L}_L^{\mathbb{R}} \;=\; \left\{ \left[\begin{pmatrix} a \\ b \end{pmatrix}\right]_\sim \;\middle|\; a,b\in \mathrm{GL}(L,\mathbb{C})\;,\;\; a^*a=b^*b\;,\;\;\; (ab^{-1})^t=ab^{-1} \right\}\;.$$

This implies that $\Pi([\Phi]_\sim)$ is symmetric for $[\Phi]_\sim \in \mathbb{L}_L^{\mathbb{R}}$. Moreover, if U in (11) is symmetric, then the last identity in (8) holds. Again Π is continuous, and Π^{-1} real analytic, so that the proof of (ii) is completed.

For case (iii), the third identity of (6) implies that the supplementary symmetry in (9) gives

$$\mathcal{C}\,\mathbb{L}_L^{\mathbb{H}} \;=\; \left\{ \left[\begin{pmatrix} a \\ b \end{pmatrix}\right]_\sim \;\middle|\; a,b\in \mathrm{GL}(L,\mathbb{C})\;,\;\; a^*a=b^*b\;,\;\;\; I^*(ab^{-1})^tI=ab^{-1} \right\}\;.$$

This implies that $I\Pi([\Phi]_\sim)$ is skew-symmetric for $[\Phi]_\sim \in \mathbb{L}_L^{\mathbb{H}}$. Again, if IU in (11) is skew-symmetric, then the last identity in (9) holds, completing the proof. □

Proof of Theorem 3. Let $\hat{\mathbb{L}}_L^{\mathbb{R}}$ and $\hat{\mathbb{L}}_L^{\mathbb{H}}$ denote the real analytic manifolds on the r.h.s. of the two equations in Theorem 3. Let us first show $\mathbb{L}_L^{\mathbb{R}} = \hat{\mathbb{L}}_L^{\mathbb{R}}$. The inclusion $\hat{\mathbb{L}}_L^{\mathbb{R}} \subset \mathbb{L}_L^{\mathbb{R}}$ is obvious because for a real representative Φ the two conditions in (8) coincide. Moreover, this inclusion is continuous. Due to Theorem 4(ii) it is sufficient to show that $\Pi^{-1}: \mathrm{U}\,(L)\cap \mathrm{Sym}(L,\mathbb{C}) \to \hat{\mathbb{L}}_L^{\mathbb{R}}$, namely that one can choose a real representative in (11). Let us use the fact that every symmetric unitary U can be diagonalized by an orthogonal matrix $M\in \mathrm{O}(L)$, namely $U=M^tDM$ where

$D = \mathrm{diag}(e^{\imath\theta_1}, \ldots, e^{\imath\theta_L})$ with $\theta_l \in [0, 2\pi)$. Now let $D^{\frac{1}{2}} = \mathrm{diag}(e^{\imath\theta_1/2}, \ldots, e^{\imath\theta_L/2})$ be calculated with the first branch of the square root and choose $S = \mathrm{diag}(\sigma_1, \ldots, \sigma_L) \in \mathrm{O}(L)$ with $\sigma_l \in \{-1, 1\}$ such that the phase of $\sigma_l e^{\imath\theta_l/2}$ is in $[0, \pi)$. Then let us introduce the unitary $V = M^t D^{\frac{1}{2}} S$. One has $U = VV^t$. Furthermore set $a = \Re e(V)$ and $b = -\Im m(V)$ and then $\Pi^{-1}(U) = [\Phi]_\sim$ with $\Phi = \begin{pmatrix} a \\ b \end{pmatrix}$. Indeed Π^{-1} is the inverse of Π:

$$\Pi([\Phi]_\sim) \;=\; \pi\left(\left[\begin{pmatrix} V \\ \overline{V} \end{pmatrix}\right]_\sim\right) \;=\; VV^t \;=\; U\;.$$

This construction of Π^{-1} was done with a bit more care than needed, but it allows to show directly that Π^{-1} is locally real analytic. Let $E \mapsto U(E)$ be a real analytic path of symmetric unitaries. Then analytic perturbation theory [Kat, Theorem II.1.10] shows that the diagonalization $U(E) = M(E)^t D(E) M(E)$ can be done with analytic $M(E)$ and $D(E)$. Furthermore $E \mapsto D(E)^{\frac{1}{2}} S(E) \in \mathrm{diag}(\mathbb{R}/\pi\mathbb{Z}, \ldots, \mathbb{R}/\pi\mathbb{Z})$ with $S(E)$ defined as above is also analytic because $\theta \in \mathbb{R}/2\pi\mathbb{Z} \mapsto \frac{\theta}{2} \in \mathbb{R}/\pi\mathbb{Z}$ is analytic. Thus $V(E) = M(E)^t D^{\frac{1}{2}}(E) S(E)$ is analytic and therefore also Π^{-1}.

The proof of $\mathbb{L}_L^{\mathbb{H}} = \hat{\mathbb{L}}_L^{\mathbb{H}}$ is just an adapted version of the usual rewriting of symplectic structures (here the symmetry induced by I and $\mathcal{I}$) in terms of quaternions. Let the basis of $\mathbb{H}$ (as real vector space) be 1 and the imaginary units $\imath, j, k$ satisfying Hamilton's equations $\imath^2 = j^2 = k^2 = \imath jk = -1$. Then $\mathbb{C}$ is identified with the span of 1 and $\imath$. Now let us introduce

$$\Upsilon \;=\; \begin{pmatrix} \mathbf{1} & j\,\mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{1} & j\,\mathbf{1} \end{pmatrix} \;\in\; \mathrm{Mat}(L \times 2L, \mathbb{H})\;,$$

where all blocks are of size $\frac{L}{2} \times \frac{L}{2}$. One readily verifies the matrix identity

$$\Upsilon^{*_{\mathbb{H}}}\, I\, \Upsilon \;=\; \mathcal{J} \;-\; j\,\mathcal{I}\;. \tag{12}$$

Hence one obtains a map $\Upsilon : \mathrm{Mat}(2L \times L, \mathbb{C}) \to \mathrm{Mat}(L \times L, \mathbb{H})$ by matrix multiplication with Υ (from the left) which induces a map on the (complex) Grassmannians of right equivalence classes. Thus due to (12) we have exhibited an analytic map $\Upsilon : \hat{\mathbb{L}}_L^{\mathbb{H}} \to \mathbb{L}_L^{\mathbb{H}}$. □

2.3 Symplectic group and Lorentz group

Let $\mathbb{K}$ be one of the fields $\mathbb{R}$, $\mathbb{C}$ and $\mathbb{H}$ and let L be even if $\mathbb{K} = \mathbb{H}$. The symplectic group $\mathrm{SP}(2L, \mathbb{K})$ is by definition the set of complex $2L \times 2L$ matrices conserving the Lagrangian structure in (7), (8) and (9) respectively, *e.g.*

$$\mathrm{SP}(2L, \mathbb{R}) \;=\; \left\{\mathcal{T} \;\in\; \mathrm{Mat}(2L, \mathbb{C}) \;|\; \mathcal{T}^* \mathcal{J} \mathcal{T} = \mathcal{J}\;,\quad \mathcal{T}^t \mathcal{J} \mathcal{T} = \mathcal{J}\;\right\}\;.$$

One verifies that $\mathcal{T} \in \mathrm{SP}(2L,\mathbb{K})$ if and only if $\mathcal{T}^* \in \mathrm{SP}(2L,\mathbb{K})$. All symplectic matrices have a unit determinant. Using the Jordan form, it can be proven that $\mathrm{SP}(2L,\mathbb{K})$ is arc-wise connected. Theorem 3 implies respectively the identity and isomorphism (direct algebraic proofs can be written out as well)

$$\mathrm{SP}(2L,\mathbb{R}) \;=\; \{\mathcal{T} \,\in\, \mathrm{Mat}(2L,\mathbb{R}) \mid \mathcal{T}^{*_{\mathbb{R}}}\mathcal{J}\mathcal{T} = \mathcal{J}\,\}\ ,$$

and

$$\mathrm{SP}(2L,\mathbb{H}) \;\cong\; \{T \,\in\, \mathrm{Mat}(L,\mathbb{H}) \mid T^{*_{\mathbb{H}}}IT = I\,\}\ .$$

More explicit formulas are given in the next algebraic lemma.

Lemma 1 *The complex symplectic group is given by*

$$\mathrm{SP}(2L,\mathbb{C}) \;=\; \left\{\left(\begin{array}{cc} A & B \\ C & D \end{array}\right) \in \mathrm{Mat}(2L,\mathbb{C})\;\middle|\; A^*C = C^*A\ ,\quad A^*D - C^*B = \mathbf{1}\ ,\quad B^*D = D^*B\right\}\ .$$

In this representation, elements of $\mathrm{SP}(2L,\mathbb{R})$ *and* $\mathrm{SP}(2L,\mathbb{H})$ *are characterized by having respectively real and self-conjugate entries* A,B,C,D*.*

As already became apparent in the proof of Theorems 3 and 4, it is convenient to use the Cayley transform. The generalized Lorentz groups are introduced by

$$\mathrm{U}(L,L,\mathbb{K}) \;=\; \mathcal{C}\,\mathrm{SP}(2L,\mathbb{K})\,\mathcal{C}^*\ .$$

¿From the identities (6) one can read off alternative definitions, *e.g.*

$$\mathrm{U}(L,L,\mathbb{R}) \;=\; \left\{\mathcal{T} \,\in\, \mathrm{Mat}(2L\times 2L,\mathbb{C}) \mid \mathcal{T}^*\,\mathcal{G}\,\mathcal{T} \;=\; \mathcal{G}\ ,\quad \mathcal{T}^t\,\mathcal{J}\,\mathcal{T} \;=\; \mathcal{J}\right\}\ .$$

Let us provide again more explicit expressions.

Lemma 2 *One has*

$$\begin{aligned}\mathrm{U}(L,L,\mathbb{C}) &= \left\{\left(\begin{array}{cc} A & B \\ C & D \end{array}\right) \in \mathrm{Mat}(2L,\mathbb{C})\;\middle|\; A^*A - C^*C = \mathbf{1}\,,\ D^*D - B^*B = \mathbf{1}\,,\ A^*B = C^*D\right\} \\ &= \left\{\left(\begin{array}{cc} A & B \\ C & D \end{array}\right) \in \mathrm{Mat}(2L,\mathbb{C})\;\middle|\; AA^* - BB^* = \mathbf{1}\,,\ DD^* - CC^* = \mathbf{1}\,,\ AC^* = BD^*\right\}.\end{aligned}$$

Furthermore, in that representation, A *and* D *are invertible and* $\|A^{-1}B\| < 1$ *and* $\|D^{-1}C\| < 1$*. For* $\mathcal{T} \in \mathrm{U}(L,L,\mathbb{R})$ *one, moreover, has* $C = \overline{B}$ *and* $D = \overline{A}$*. For* $\mathcal{T} \in \mathrm{U}(L,L,\mathbb{H})$ *the entries satisfy* $C = I^*\overline{B}I$ *and* $D = I^*\overline{A}I$*.*

Proof. The first relations are equivalent to $\mathcal{T}^*\mathcal{G}\mathcal{T} = \mathcal{G}$, the second ones then follow from the fact that $\mathcal{T}^* \in \mathrm{U}(L,L,\mathbb{C})$ for $\mathcal{T} \in \mathrm{U}(L,L,\mathbb{C})$. The fact that A is invertible follows from $AA^* \geq \mathbf{1}$. Furthermore $AA^* - BB^* = \mathbf{1}$ implies that $A^{-1}B(A^{-1}B)^* = \mathbf{1} - A^{-1}(A^{-1})^* < \mathbf{1}$, so that $\|A^{-1}B\| < 1$. The same argument applies to D and $D^{-1}C$. The last two statements can be checked by a short calculation. $\square$

2.4 Upper half-planes and Cartan's classical domains

The upper half-plane and unit disc are defined by

$$\mathbb{U}_L^{\mathbb{C}} \;=\; \{Z \in \mathrm{Mat}(L \times L, \mathbb{C}) \mid \imath(Z^* - Z) > 0 \;\}\;, \quad \mathbb{D}_L^{\mathbb{C}} \;=\; \{U \in \mathrm{Mat}(L \times L, \mathbb{C}) \mid U^*U < \mathbf{1} \;\}\;,$$

where $Y > 0$ means that Y is positive definite. Furthermore let us introduce the following subsets (here L does not need to be even for $\mathbb{K} = \mathbb{H}$):

$$\mathbb{U}_L^{\mathbb{R}} \;=\; \mathbb{U}_L^{\mathbb{C}} \cap \mathrm{Sym}(L, \mathbb{C})\;, \qquad \mathbb{U}_L^{\mathbb{H}} \;=\; \mathbb{U}_L^{\mathbb{C}} \cap \mathrm{Self}(L, \mathbb{C})\;,$$

and

$$\mathbb{D}_L^{\mathbb{R}} \;=\; \mathbb{D}_L^{\mathbb{C}} \cap \mathrm{Sym}(L, \mathbb{C})\;, \qquad \mathbb{D}_L^{\mathbb{H}} \;=\; \mathbb{D}_L^{\mathbb{C}} \cap \mathrm{Self}(L, \mathbb{C})\;.$$

Let us note that $I\mathbb{D}_L^{\mathbb{H}} = \mathbb{D}_L^{\mathbb{C}} \cap \mathrm{Skew}(L, \mathbb{C})$. The sets $\mathbb{D}_L^{\mathbb{C}}$, $\mathbb{D}_L^{\mathbb{R}}$ and $I\mathbb{D}_L^{\mathbb{H}}$ are called Cartan's first, second and third classical domain [Hua]. Furthermore $\mathbb{U}_L^{\mathbb{R}}$ and $\mathbb{D}_L^{\mathbb{R}}$ are also called the Siegel upper half-plane and the Siegel disc [Sie]. The Cayley transform maps (via Möbius transformation) the upper half-planes bijectively to the generalized unit discs, as shown next.

Proposition 1 *The formulas*

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

establish an analytic diffeomorphism from $\mathbb{U}_L^{\mathbb{K}}$ onto $\mathbb{D}_L^{\mathbb{K}}$ for $\mathbb{K} = \mathbb{C}, \mathbb{R}, \mathbb{H}$.

Proof. (*cf.* [Sie]; reproduced for the convenience of the reader.) If $v \in \ker(Z + \imath\mathbf{1})$, then $\imath v = -Zv$ so that $0 \leq \langle v|\imath(Z^* - Z)|v\rangle = -2\,\langle v|v\rangle$ which implies $v = 0$. Hence $Z + \imath\mathbf{1}$ is invertible and the first formula is well-defined. Similarly one checks the invertibility of $\mathbf{1} - U$. To verify that one is the inverse of the other is a matter of calculation. Moreover, both formulas preserve the symmetry and self-duality of the matrices involved. □

The boundary $\partial\mathbb{U}_L^{\mathbb{C}}$ of $\mathbb{U}_L^{\mathbb{C}}$ is a stratified space given as the union of strata $\partial_l\mathbb{U}_L^{\mathbb{C}}$, $l = 1, \ldots, L$, where $\partial_l\mathbb{U}_L^{\mathbb{C}}$ is the set of matrices Z for which $\imath(Z^* - Z) \geq 0$ is of rank $L - l$. The maximal boundary is $\partial_L\mathbb{U}_L^{\mathbb{C}}$ are the selfadjoint matrices. Furthermore $\partial\mathbb{U}_L^{\mathbb{R}} = \partial\mathbb{U}_L^{\mathbb{C}} \cap \mathrm{Sym}(L, \mathbb{C})$ with strata $\partial_l\mathbb{U}_L^{\mathbb{R}} = \partial_l\mathbb{U}_L^{\mathbb{C}} \cap \mathrm{Sym}(L, \mathbb{C})$. Corresponding formulas hold for $\mathbb{K} = \mathbb{H}$.

Similarly the boundary $\partial\mathbb{D}_L^{\mathbb{C}}$ is a stratified space with strata $\partial_l\mathbb{D}_L^{\mathbb{C}}$, $l = 1, \ldots, L$, of matrices U for which $U^*U \leq \mathbf{1}$ and $\mathrm{rank}(\mathbf{1} - U^*U) = L - l$. For $\mathbb{K} = \mathbb{R}, \mathbb{H}$ one defines in the same way the stratified boundaries $\partial\mathbb{D}_L^{\mathbb{K}} = \cup_{l=1}^{L}\partial_l\mathbb{D}_L^{\mathbb{K}}$. Of particular importance will be the maximal boundaries (L even for $\mathbb{K} = \mathbb{H}$):

$$\partial_L\mathbb{D}_L^{\mathbb{C}} \;=\; \mathrm{U}(L)\;, \qquad \partial_L\mathbb{D}_L^{\mathbb{R}} \;=\; \mathrm{U}(L) \cap \mathrm{Sym}(L, \mathbb{C})\;, \qquad \partial_L\mathbb{D}_L^{\mathbb{H}} \;=\; \mathrm{U}(L) \cap \mathrm{Self}(L, \mathbb{C})\;.$$

By Theorem 4 the maximal boundary $\partial_L\mathbb{D}_L^{\mathbb{K}}$ is hence identified with the Lagrangian Grassmannian $\mathbb{L}_L^{\mathbb{K}}$. Let us also note that the Cayley transformation of Proposition 1 has singularities on the boundaries and mixes the strata. In particular, $\partial_L\mathbb{U}_L^{\mathbb{K}}$ is not mapped to $\partial_L\mathbb{D}_L^{\mathbb{K}}$.

2.5 Möbius action

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

$$\mathcal{T}\cdot Z \;=\; (AZ+B)\,(CZ+D)^{-1}\;, \qquad \mathcal{T}\;=\;\begin{pmatrix} A & B \\ C & D \end{pmatrix}\;\in\;\mathrm{GL}(2L,\mathbb{C})\;,\;\; Z\in\mathrm{Mat}(L\times L,\mathbb{C})\;, \tag{13}$$

whenever the appearing inverse exists. This action implements the matrix multiplication, namely

$$\pi\big(\mathcal{T}([\Phi]_\sim)\big)\;=\;\mathcal{T}\cdot\pi\big([\Phi]_\sim\big)\;, \qquad \text{if}\;\;[\Phi]_\sim\in\mathbb{G}_L^{\mathrm{inv}}\;\text{and}\;\;[\mathcal{T}\Phi]_\sim\in\mathbb{G}_L^{\mathrm{inv}}\;. \tag{14}$$

Indeed, let $\Phi=\begin{pmatrix} a \\ b \end{pmatrix}$. Then $[\mathcal{T}\Phi]_\sim\in\mathbb{G}_L^{\mathrm{inv}}$ implies that $Ca+Db$ is invertible. As b is invertible (because $[\Phi]_\sim\in\mathbb{G}_L^{\mathrm{inv}}$), it follows that $Cab^{-1}+D=C\pi([\Phi]_\sim)+D$ is invertible so that the Möbius transformation $\mathcal{T}\cdot\pi\big([\Phi]_\sim\big)$ is well-defined. The conditions in (14) are automatically satisfied in the situation of the following proposition. The proof of item (ii) is contained in the proof of Theorem 5 below; item (i) then follows directly from (ii) due to Proposition 1.

Proposition 2 [Hua, Sie] *Let $\mathbb{K}=\mathbb{C},\mathbb{R},\mathbb{H}$ and let L be even for $\mathbb{K}=\mathbb{H}$.*
(i) $\mathrm{SP}(2L,\mathbb{K})$ *acts on $\mathbb{U}_L^{\mathbb{K}}$ by Möbius transformation.*
(ii) $\mathrm{U}(L,L,\mathbb{K})$ *acts on $\mathbb{D}_L^{\mathbb{K}}$ by Möbius transformation.*

The following proposition states that the action of Proposition 2(ii) extends to the stratified boundary of $\mathbb{D}_L^{\mathbb{K}}$. Moreover, the action on the maximal boundary $\partial_L\mathbb{D}_L^{\mathbb{K}}$ implements the natural action of the symplectic group on the Lagrangian Grassmannian. Due to singularities it is not possible to extend the action of Proposition 2(i) to any stratum of the boundary of $\mathbb{U}_L^{\mathbb{K}}$.

Theorem 5 *Let $\mathbb{K}=\mathbb{C},\mathbb{R},\mathbb{H}$ and L even if $\mathbb{K}=\mathbb{H}$ and $l=1,\ldots,L$. The Lorentz group* $\mathrm{U}(L,L,\mathbb{K})$ *acts on $\partial_l\mathbb{D}_L^{\mathbb{K}}$ by Möbius transformation. For the case $l=L$ of the maximal boundary, this action implements the action of* $\mathrm{SP}(2L,\mathbb{K})$ *on the Lagrangian Grassmannian $\mathbb{L}_L^{\mathbb{K}}$:*

$$\Pi\big([\mathcal{T}\Phi]_\sim\big)\;=\;\mathcal{C}\,\mathcal{T}\,\mathcal{C}^*\cdot\Pi\big([\Phi]_\sim\big)\;, \qquad [\Phi]_\sim\in\mathbb{L}_L^{\mathbb{K}}\;,\quad \mathcal{T}\in\;\mathrm{SP}(2L,\mathbb{K})\;.$$

Proof. One has to show that for $U\in\partial_l\mathbb{D}_L^{\mathbb{K}}$ and $\mathcal{T},\mathcal{T}'\in\mathrm{U}(L,L,\mathbb{C})$ the Möbius transformation $\mathcal{T}\cdot U$ is well-defined, is again in $\partial_l\mathbb{D}_L^{\mathbb{K}}$ and that $(\mathcal{T}\mathcal{T}')\cdot U=\mathcal{T}\cdot(\mathcal{T}'\cdot U)$. Let $\mathcal{T}$ be given in terms of A,B,C,D as in Lemma 2. Then this lemma implies that $(CU+D)=D(\mathbf{1}+D^{-1}CU)$ is invertible so that the Möbius transform is well-defined. Let us first show that $(\mathcal{T}\cdot U)^*(\mathcal{T}\cdot U)\leq\mathbf{1}$. For this purpose, one can appeal to the identity

$$(C\,U\,+\,D)^*\,(C\,U\,+\,D)\;-\;(A\,U\,+\,B)^*\,(A\,U\,+\,B)\;=\;\mathbf{1}\;-\;U^*\,U\;, \tag{15}$$

following directly from the identities in Lemma 2. Indeed, multiplying (15) from the left by $((CU+D)^*)^{-1}$ and the right by $(CU+D)^{-1}$ and using $\mathbf{1}-U^*U \geq \mathbf{0}$ shows $(\mathcal{T}\cdot U)^*(\mathcal{T}\cdot U) \leq \mathbf{1}$. Next let us show that the invertible $(CU+D)$ maps $\ker(\mathbf{1}-U^*U)$ to $\ker(\mathbf{1}-(\mathcal{T}\cdot U)^*(\mathcal{T}\cdot U))$ and $\ker(\mathbf{1}-U^*U)^\perp$ to $\ker(\mathbf{1}-(\mathcal{T}\cdot U)^*(\mathcal{T}\cdot U))^\perp$. If $v \in \ker(\mathbf{1}-U^*U)$, then (15) implies

$$\|(CU+D)\,v\| \;=\; \|(AU+B)\,v\| \;=\; \|\mathcal{T}\cdot U\,(CU+D)\,v\|\,,$$

so that $(CU+D)v \in \ker(\mathbf{1}-(\mathcal{T}\cdot U)^*(\mathcal{T}\cdot U))$ because $\mathbf{1}-(\mathcal{T}\cdot U)^*(\mathcal{T}\cdot U) \geq 0$. Similarly for $v \in \ker(\mathbf{1}-U^*U)^\perp$ one has $\|(CU+D)v\| > \|\mathcal{T}\cdot U(CU+D)v\|$ implying that $v \notin \ker(\mathbf{1}-(\mathcal{T}\cdot U)^*(\mathcal{T}\cdot U))$.

The argument up to now shows that $\mathcal{T}\cdot U \in \partial_l \mathbb{D}_L^{\mathbb{C}}$. A short algebraic calculation also shows that $(\mathcal{T}\mathcal{T}')\cdot Z = \mathcal{T}\cdot(\mathcal{T}'\cdot Z)$. It remains to show that the symmetries are conserved in the cases $\mathbb{K}=\mathbb{R},\mathbb{H}$. For $\mathcal{T}\in U(L,L,\mathbb{R})$ one has $C=\overline{B}$ and $D=\overline{A}$ by Lemma 2, so that

$$\mathcal{T}\cdot U-(\mathcal{T}\cdot U)^t \;=\; ((\overline{B}U+\overline{A})^{-1})^t\left[(\overline{B}U+\overline{A})^t(AU+B)-(AU+B)^t(\overline{B}U+\overline{A})\right](\overline{B}U+\overline{A})^{-1}\,.$$

For symmetric U one checks that the term in the bracket vanishes due to the identities in Lemma 2, implying that $\mathcal{T}\cdot U$ is again symmetric. Similarly one proceeds in the case $\mathbb{K}=\mathbb{H}$.

Now let us come to the last point of the proposition. Given $U \in \partial_L\mathbb{D}_L^{\mathbb{K}}$, let $[\Phi]_\sim \in \mathbb{L}_L^{\mathbb{K}}$ be such that $\Pi([\Phi]_\sim)=U$ (by the construction in the proof of Theorem 4). For $\mathcal{T}\in \mathrm{SP}(2L,\mathbb{K})$, one then has $[\mathcal{T}\Phi]_\sim \in \mathbb{L}_L^{\mathbb{K}}$. Theorem 4 implies that both $[\mathcal{C}\Phi]_\sim$ and $[\mathcal{C}\mathcal{T}\Phi]_\sim=[\mathcal{C}\mathcal{T}\mathcal{C}^*\mathcal{C}\Phi]_\sim$ are in $\mathbb{G}_L^{\mathrm{inv}}$. From (14) now follows that $\mathcal{C}\mathcal{T}\mathcal{C}^*\cdot\pi([\mathcal{C}\Phi]_\sim)=\pi([\mathcal{C}\mathcal{T}\Phi]_\sim)$. □

It is interesting to note (and relevant for Section 3.6) that the Möbius transformation sends $\mathbb{U}_L^{\mathbb{K}}$ to $\mathbb{U}_L^{\mathbb{K}}$ for some complex matrices in $\mathrm{GL}(2L,\mathbb{C})$ which are not in $\mathrm{SP}(2L,\mathbb{K})$. In particular, for $\delta>0$ one even has:

$$\begin{pmatrix}\mathbf{1} & \imath\,\delta\,\mathbf{1}\\ \mathbf{0} & \mathbf{1}\end{pmatrix}\cdot Z \;=\; Z+\imath\,\delta\,\mathbf{1}\;\in\;\mathbb{U}_L^{\mathbb{K}}\,,\qquad \text{for}\;\; Z\in\mathbb{U}_L^{\mathbb{K}}\cup\partial\mathbb{U}_L^{\mathbb{K}}\,. \tag{16}$$

The following formula shows that the Möbius transformation appears naturally in the calculation of a volume distortion by an invertible matrix, namely the so-called Radon-Nykodym cocycle. It will be used for the calculation of the sum of Lyapunov exponents in Section 4.1.

Lemma 3 *Suppose that* $[\Phi]_\sim\in\mathbb{G}_L^{\mathrm{inv}}$ *and* $[\mathcal{T}\Phi]_\sim\in\mathbb{G}_L^{\mathrm{inv}}$ *where* $\mathcal{T}\in\mathrm{GL}(2L,\mathbb{C})$*. With notations for* $\mathcal{T}$ *as in* (13) *one has*

$$\frac{\det\big((\mathcal{T}\Phi)^*(\mathcal{T}\Phi)\big)}{\det\big(\Phi^*\Phi\big)} \;=\; \frac{\det\big((\mathcal{T}\cdot\pi([\Phi]_\sim))^*(\mathcal{T}\cdot\pi([\Phi]_\sim))+\mathbf{1}\big)}{\det\big((\pi([\Phi]_\sim))^*(\pi([\Phi]_\sim))+\mathbf{1}\big)}\;\Big|\det\big(C\,\pi([\Phi]_\sim)+D\big)\Big|^2\,.$$

Proof. Let $\Phi = \begin{pmatrix} a \\ b \end{pmatrix}$. As b is invertible by hypothesis,

$$\frac{\det\big((\mathcal{T}\Phi)^*(\mathcal{T}\Phi)\big)}{\det\big(\Phi^*\Phi\big)} = \frac{\det\big((Aab^{-1}+B)^*(Aab^{-1}+B)+(Cab^{-1}+D)^*(Cab^{-1}+D)\big)}{\det\big((ab^{-1})^*(ab^{-1})+\mathbf{1}\big)} .$$

Furthermore, it was supposed that $Cab^{-1}+D$ is also invertible, and this allows to conclude the proof because $\pi([\Phi]_\sim) = ab^{-1}$. □

2.6 Singular cycles

Given $\xi \in \mathrm{Sym}(L,\mathbb{R}) \cap \mathrm{Self}(L,\mathbb{C})$, let us set $\Psi_\xi = \begin{pmatrix} \xi \\ \mathbf{1} \end{pmatrix}$. The associated singular cycle (often called Maslov cycle, but it actually already appears in Bott's work [Bot]) is

$$\mathbb{L}_L^{\mathbb{K},\xi} = \Big\{ [\Phi]_\sim \in \mathbb{L}_L^{\mathbb{K}} \;\Big|\; \Phi\,\mathbb{C}^L \cap \Psi_\xi\,\mathbb{C}^L \neq \{\vec{0}\} \Big\} .$$

It can be decomposed into a disjoint union of $\mathbb{L}_L^{\mathbb{K},\xi,l}$, $l = 1,\ldots,L$, where

$$\mathbb{L}_L^{\mathbb{K},\xi,l} = \big\{ [\Phi]_\sim \in \mathbb{L}_L^{\mathbb{K}} \;\big|\; \dim\big(\Phi\,\mathbb{C}^L \cap \Psi_\xi\,\mathbb{C}^L\big) = l \big\} .$$

It is possible to define singular cycles associated to Lagrangian planes which are not of the form of Ψ_ξ, but this will not be used here.

It is convenient to express the intersection conditions in terms of the Wronskian associated to two $2L \times L$ matrices Φ and Ψ representing two Lagrangian planes

$$W(\Phi,\Psi) = \Phi^* \mathcal{J} \Psi ,$$

namely one checks that $\Phi\,\mathbb{C}^L \cap \Psi\,\mathbb{C}^L \neq \{\vec{0}\} \Leftrightarrow \det\big(W(\Phi,\Psi)\big) = 0$, and, more precisely,

$$\dim\big(\Phi\,\mathbb{C}^L \cap \Psi\,\mathbb{C}^L\big) = \dim\big(\ker W(\Phi,\Psi)\big) . \tag{17}$$

Note that even though $W(\Phi,\Psi)$ does depend on the choice of basis in the two Lagrangian planes, the dimension of its kernel is independent of this choice. Furthermore, $W(\Phi,\Psi) = \mathbf{0}$ if and only if $[\Phi]_\sim = [\Psi]_\sim$.

Arnold showed in [Arn1] that $\mathbb{L}_L^{\mathbb{R},\xi}$ is two-sided by exhibiting a non-vanishing transversal vector field on $\mathbb{L}_L^{\mathbb{R},\xi}$. This allows to define a weighted intersection number for paths in a generic position, namely for paths having only intersections with the highest stratum $\mathbb{L}_L^{\mathbb{R},\xi,1}$. Bott proved a similar result for $\mathbb{L}_L^{\mathbb{C},\xi}$ already earlier [Bot]. Using the following proposition, it will be straightforward in the next section to define intersection numbers for paths which are not necessarily in a generic position.

Proposition 3 $\Pi(\mathbb{L}_L^{\mathbb{K},\xi,l}) = \partial_L^{\xi,l}\mathbb{D}_L^{\mathbb{K}}$ *where* $\partial_L^{\xi,l}\mathbb{D}_L^{\mathbb{K}}$ *is the following subset of the maximal boundary* $\partial_L\mathbb{D}_L^{\mathbb{K}}$*:*

$$\partial_L^{\xi,l}\mathbb{D}_L^{\mathbb{K}} \;=\; \left\{ U \in \partial_L\mathbb{D}_L^{\mathbb{K}} \;|\; \mathrm{rank}\,(\Pi([\Psi_\xi]_\sim) - U) \;=\; L - l \right\} .$$

Setting $\partial_L^{\xi}\mathbb{D}_L^{\mathbb{K}} = \cup_{l=1,\ldots,L}\,\partial_L^{\xi,l}\mathbb{D}_L^{\mathbb{K}}$*, one has* $\Pi(\mathbb{L}_L^{\mathbb{K},\xi}) = \partial_L^{\xi}\mathbb{D}_L^{\mathbb{K}}$*. One has* $\mathbf{1} \notin \partial_L^{\xi}\mathbb{D}_L^{\mathbb{K}}$ *for any* $\xi \in \mathrm{Sym}(L,\mathbb{R}) \cap \mathrm{Self}(L,\mathbb{R})$.

Proof. Given U, let $\Phi = \begin{pmatrix} a \\ b \end{pmatrix}$ where $a = \frac{1}{2}(U + \mathbf{1})$ and $b = \frac{\imath}{2}(U - \mathbf{1})$ as in the proof of Theorem 4. Hence $\Pi([\Phi]_\sim) = U$. Then one verifies

$$W(\Psi_\xi, \Phi) \;=\; a \,-\, \xi\, b \;=\; \frac{1}{2}\left(U \,+\, \mathbf{1} \,-\, \imath\,\xi\,(U \,-\, \mathbf{1})\right) \;=\; \frac{1}{2}\,(\mathbf{1} - \imath\,\xi)\left(U \,-\, \Pi([\Psi_\xi]_\sim)\right) .$$

As $\mathbf{1} - \imath\,\xi$ is invertible, the result follows directly from (17). No more care is needed in the real case because the dimension of the kernel of the Wronskian is independent of a basis change from the above Φ to the real one in the proof of Theorem 4. $\Box$

We will only use the singular cycles associated to $\xi = -\cot(\frac{\varphi}{2})\,\mathbf{1}$ where $\varphi \in (0, 2\pi)$, and only need to use $\mathbb{K} = \mathbb{C}$ as the supplementary symmetries are irrelevant for the definition and calculation of the intersection number (Bott or Maslov index) in the next sections. Let us denote these singular cycles, subsets of $\mathbb{L}_L^{\mathbb{C}}$, by $\mathbb{L}_L^{\varphi} = \cup_{l=1,\ldots,L}\mathbb{L}_L^{\varphi,l}$. The image under Π will then be written as $\partial_L^{\varphi}\mathbb{D}_L^{\mathbb{C}} = \cup_{l=1,\ldots,L}\partial_L^{\varphi,l}\mathbb{D}_L^{\mathbb{C}}$. Because $\Pi(\Psi_\xi) = e^{\imath\varphi}\mathbf{1}$, it follows from Proposition 3 that

$$\Pi(\mathbb{L}_L^{\varphi,l}) \;=\; \partial_L^{\varphi,l}\mathbb{D}_L^{\mathbb{C}} \;=\; \{\, U \in \mathrm{U}(L) \;|\; e^{\imath\varphi} \text{ eigenvalue of } U \text{ with multiplicity } l \,\} . \qquad (18)$$

2.7 The intersection number (Bott index)

Let $\Gamma = ([\Phi^E]_\sim)_{E\in[E_0,E_1)}$ be a (continuous) closed path in $\mathbb{L}_L^{\mathbb{C}}$ for which the number of intersections $\{E \in [E_0, E_1) \;|\; \Gamma(E) \in \mathbb{L}_L^{\varphi}\}$ is finite. At an intersection $\Gamma(E) \in \mathbb{L}_L^{\varphi,l}$, let $\theta_1(E'), \ldots, \theta_l(E')$ be those eigenphases of the unitary $\Pi(\Gamma(E'))$ which are all equal to φ at $E' = E$. Choose $\epsilon, \delta > 0$ such that $\theta_k(E') \in [\varphi - \delta, \varphi + \delta]$ for $k = 1, \ldots, l$ and $E' \in [E - \epsilon, E + \epsilon]$ and that there are no other eigenphases in $[\varphi - \delta, \varphi + \delta]$ for $E' \neq E$ and finally $\theta_k(E') \neq \varphi$ for those parameters. Let n_- and n_+ be the number of those of the l eigenphases less than φ respectively before and after the intersection, and similarly let p_- and p_+ be the number of eigenphases larger than φ before and after the intersection. Then the signature of $\Gamma(E)$ is defined by

$$\mathrm{sgn}(\Gamma(E)) \;=\; \frac{1}{2}\,(p_+ - n_+ - p_- + n_-) \;=\; l - n_+ - p_- . \qquad (19)$$

Note that $-l \leq \mathrm{sgn}(\Gamma(E)) \leq l$ and that $\mathrm{sgn}(\Gamma(E))$ is the effective number of eigenphases that have crossed φ in the counter-clock sense. Furthermore the signature is stable under perturbations of the path in the following sense: if an intersection by $\mathbb{L}_L^{\varphi,l}$ is resolved by a perturbation into a series of intersections by lower strata, then the sum of their signatures is equal to $\mathrm{sgn}(\Gamma(E))$. Finally let us remark that, if the phases are differentiable and $\partial_E\theta_k(E)\neq 0$ for $k=1,\ldots,l$, then $\mathrm{sgn}(\Gamma(E))$ is equal to the sum of the l signs $\mathrm{sgn}(\partial_E\theta_k(E))$, $k=1,\ldots,l$. Now the intersection number or index of the path Γ w.r.t. the singular cycle $\mathbb{L}_L^\varphi$ is defined by

$$\mathrm{ind}(\Gamma,\mathbb{L}_L^\varphi) \;=\; \sum_{\Gamma(E)\,\in\,\mathbb{L}_L^\varphi} \mathrm{sgn}(\Gamma(E))\;. \tag{20}$$

Let us give a different expression for this index. If $E\in[E_0,E_1]\mapsto\theta_l^E$ are continuous paths of the eigenphases of $\Pi(\Gamma(E))$ with arbitrary choice of enumeration at level crossings, then each of them leads to a winding number. A bit of thought shows that

$$\mathrm{ind}(\Gamma,\mathbb{L}_L^\varphi) \;=\; \sum_{l=1}^{L} \mathrm{Wind}\Big(\,E\in[E_0,E_1)\mapsto\theta_l^E\,\Big)\;. \tag{21}$$

In particular, the r.h.s. is independent of the choice of enumeration at level crossings. Moreover, for the r.h.s. to make sense, one does not need to impose that the number of intersections is finite, as is, of course, necessary in order to define an intersection number. Similarly, the index of a closed path Γ in the real or quaternion Lagrangian Grassmannian could be defined; however, this index coincides with $\mathrm{ind}(\Gamma,\mathbb{L}_L^\varphi)$ if Γ is considered as path in the complex Lagrangian Grassmannian.

In the literature, $\mathrm{ind}(\Gamma,\mathbb{L}_L^\varphi)$ is often referred to as the Maslov index, at least in the case of a path in $\mathbb{L}_L^{\mathbb{R}}$. The same object already appears in the work of Bott [Bot] though, and it seems more appropriate to associate his name to it. The above definition using (19) appears to be considerably more simple, and the author does not know whether it was already used elsewhere.

2.8 Arnold's cocycle

Arnold has shown [Arn1] that $H^1(\mathbb{L}_L^{\mathbb{R}},\mathbb{Z})\cong\mathbb{Z}$. This and $H^1(\mathbb{L}_L^{\mathbb{K}},\mathbb{Z})\cong\mathbb{Z}$ follows from Theorem 4. The generator ω of the de Rahm groups can be chosen as follows. A continuous closed path $\Gamma=([\Phi^E]_\sim)_{E\in[E_0,E_1)}$ in $\mathbb{L}_L^{\mathbb{C}}$ gives rise to a continuous closed path $E\in[E_0,E_1)\mapsto\det(\Pi([\Phi^E]_\sim))$ in S^1. Its winding number defines the pairing of (the de Rahm class of) ω with the (homotopy class of the) path Γ:

$$\langle\,\omega\,|\,\Gamma\,\rangle \;=\; \mathrm{Wind}\Big(\,E\in[E_0,E_1)\mapsto\det(\Pi([\Phi^E]_\sim))\,\Big)\;.$$

Any continuous path in $\mathbb{L}_L^{\mathbb{C}}$ can be approximated by a differentiable one, hence we suppose from now on that Γ is differentiable. Then one can calculate the pairing by

$$\langle\, \omega \,|\, \Gamma\, \rangle \;=\; \int_{E_0}^{E_1} \frac{dE}{2\pi}\; \Im m\; \partial_E\; \log(\det(\Pi([\Phi^E]_\sim)))\;. \tag{22}$$

The next theorem is Arnold's main result concerning this cycle.

Theorem 6 [Arn1] *Provided a closed differentiable path* Γ *has only finitely many intersections with the singular cycle* $\mathbb{L}_L^{\varphi}$*,*

$$\mathrm{ind}(\Gamma, \mathbb{L}_L^{\varphi}) \;=\; \langle\, \omega \,|\, \Gamma\, \rangle\;.$$

Proof. Set $U(E) = \Pi(\Gamma(E))$. As already used in the proof of Theorem 4, the diagonalization $U(E) = M(E)^* D(E) M(E)$ can be done with a differentiable unitary matrix $M(E)$ and a differentiable diagonal matrix $D(E) = \mathrm{diag}(e^{\imath\theta_1^E}, \ldots, e^{\imath\theta_L^E})$. As $M^E(\partial_E M^E)^* = -(\partial_E M^E)(M^E)^*$, one has

$$\Im m\; \partial_E\; \log(\det(U(E))) \;=\; \frac{1}{\imath}\,\mathrm{Tr}\,((D(E))^* \partial_E D(E)) \;=\; \sum_{l=1}^{L}\; \partial_E\, \theta_l^E\;.$$

Integrating w.r.t. E as in (22) hence shows that $\langle\, \omega \,|\, \Gamma\, \rangle$ is equal to the sum of the winding numbers of the eigenphases and this is equal to the index by (21). $\Box$

Remark It follows from the Gohberg-Krein index theorem that the intersection number is also equal to the Fredholm index of an associated Toeplitz operator [BS].

If $\mathcal{T} \in \mathrm{SP}(2L, \mathbb{C})$, then one can define another closed path in $\mathbb{L}_L^{\mathbb{C}}$ by $\mathcal{T}\Gamma = ([\mathcal{T}\Phi^E]_\sim)_{E\in[E_0,E_1)}$. Because $\mathrm{SP}(2L, \mathbb{C})$ is arc-wise connected, it follows from the homotopy invariance of the pairing that $\langle\, \omega \,|\, \mathcal{T}\Gamma\, \rangle = \langle\, \omega \,|\, \Gamma\, \rangle$. The following proposition allows $\mathcal{T}$ to vary and also analyzes intermediate values of the integral in (22), denoted by:

$$\int_{\Gamma}^{E} \omega \;=\; \int_{E_0}^{E} \frac{de}{2\pi}\; \Im m\; \partial_e\; \log(\det(\Pi([\Phi^e]_\sim)))\;, \qquad E \in [E_0, E_1)\;.$$

Proposition 4 *Let* $\Gamma = ([\Phi^E]_\sim)_{E\in[E_0,E_1)}$ *be a closed differentiable path in* $\mathbb{L}_L^{\mathbb{C}}$ *and* $(\mathcal{T}^E)_{E\in[E_0,E_1)}$ *be a differentiable path in* $\mathrm{SP}(2L, \mathbb{C})$ *such that* $\Gamma' = ([\mathcal{T}^E\Phi]_\sim)_{E\in[E_0,E_1)}$ *is a closed path in* $\mathbb{L}_L^{\mathbb{C}}$ *for any given* $[\Phi]_\sim \in \mathbb{L}_L^{\mathbb{C}}$*. Furthermore let us introduce the closed path* $\Gamma'' = ([\mathcal{T}^E\Phi^E]_\sim)_{E\in[E_0,E_1)}$*. Then*

$$\langle\, \omega \,|\, \Gamma''\, \rangle \;=\; \langle\, \omega \,|\, \Gamma\, \rangle \;+\; \langle\, \omega \,|\, \Gamma'\, \rangle\;.$$

Furthermore, with the notation

$$\mathcal{C}\,\mathcal{T}^E\,\mathcal{C}^* \;=\; \begin{pmatrix} A^E & B^E \\ C^E & D^E \end{pmatrix}\,,$$

one has (independent of $[\Phi]_\sim$*)*

$$\langle\,\omega\,|\,\Gamma'\,\rangle \;=\; \int_{E_0}^{E_1}\frac{dE}{2\,\pi}\,\Im m\;\partial_E\;\log\bigl(\det(A^E(D^E)^{-1})\bigr)\;, \tag{23}$$

and, uniformly in E*,*

$$\Bigl|\,\int_{\Gamma''}^{E}\omega\;-\;\int_{\Gamma}^{E}\omega\;-\;\int_{E_0}^{E}\frac{de}{2\,\pi}\,\Im m\;\partial_e\;\log\bigl(\det(A^e(D^e)^{-1})\bigr)\,\Bigr|\;\leq\;L\;.$$

Proof. Set $U^e=\Pi([\Phi^e]_\sim)$. Due to Theorem 5,

$$\int_{\Gamma''}^{E}\omega\;=\;\int_{E_0}^{E}\frac{de}{2\pi}\;\Im m\;\partial_e\Bigl(\;\log(\det(A^e\,U^e+B^e))-\log(\det(C^e\,U^e+D^e\,))\;\Bigr)\;.$$

In the first contribution, let us use $\det(A^e\,U^e+B^e)=\det(B^e\,(U^e)^*+A^e)\det(U^e)$, of which the second factor leads to $\int_\Gamma^E\omega$. Hence

$$\int_{\Gamma''}^{E}\omega\;-\;\int_{\Gamma}^{E}\omega\;=\;\int_{E_0}^{E}\frac{de}{2\,\pi}\;\Im m\;\partial_e\;(\log(\det(B^e\,(U^e)^*+A^e))-\log(\det(C^e\,U^e+D^e\,)))\;\;.$$

Now A^e and D^e are invertible due to Lemma 2. Hence

$$\begin{aligned}&\int_{\Gamma''}^{E}\omega\;-\;\int_{\Gamma}^{E}\omega\;-\;\int_{E_0}^{E}\frac{de}{2\,\pi}\;\Im m\;\partial_e\;\log\bigl(\det(A^e(D^e)^{-1})\bigr)\\&\qquad=\;\int_{E_0}^{E}\frac{de}{2\,\pi}\,\partial_e\;\Im m\;\Bigl(\;\mathrm{Tr}\,\bigl(\log(\mathbf{1}+(A^e)^{-1}B^e\,(U^e)^*)\bigr)-\mathrm{Tr}\,\bigl(\log(\mathbf{1}+(D^e)^{-1}C^e\,U^e)\bigr)\;\Bigr)\;.\end{aligned}$$

As $\|(A^e)^{-1}B^e\|\,<\,1$ and $\|(D^e)^{-1}C^e\|\,<\,1$ by Lemma 2, only one branch of the logarithm is needed. As $E\to E_1$ this term therefore vanishes implying the result on the winding numbers because the third term on the l.h.s. then gives $\langle\,\omega\,|\,\Gamma'\,\rangle$ as one sees repeating the above arguments with U^e replaced by the constant $\Pi([\Phi]_\sim)$. Moreover, one may carry out the integral on the r.h.s. of the last equation using the fundamental theorem, so that this r.h.s. is equal to

$$\frac{1}{2\,\pi}\;\Bigl(\;\mathrm{Tr}\,\bigl(\log(\mathbf{1}+(A^E)^{-1}B^E\,(U^E)^*)\bigr)-\mathrm{Tr}\,\bigl(\log(\mathbf{1}+(D^E)^{-1}C^E\,U^E)\bigr)\;\Bigr)\;.$$

The bound follows now from the spectral mapping theorem for the logarithm function. □

In order to calculate the integral in (22), one can also appeal to the following formula.

Lemma 4 *If $E \mapsto \Phi^E$ is differentiable and $[\Phi^E]_\sim \in \mathbb{L}_L^{\mathbb{C}}$, then*

$$\Im m\ \partial_E\ \log(\det(\Pi([\Phi^E]_\sim)))\ =\ 2\,\mathrm{Tr}\Big(\ \big((\Phi^E)^*\Phi^E\big)^{-1}\,(\Phi^E)^*\,\mathcal{J}\,(\partial_E\,\Phi^E)\Big)\ . \tag{24}$$

Proof. As in the proof of Theorem 6, let us begin with the identity

$$\imath\,\partial_E\ \log(\det(\Pi([\Phi^E]_\sim)))\ =\ \mathrm{Tr}\Big(\ (\Pi([\Phi^E]_\sim))^*\,(\partial_E\,\Pi([\Phi^E]_\sim))\ \Big)\ . \tag{25}$$

Introducing the invertible $L \times L$ matrices

$$\phi_\pm^E\ =\ (\,\mathbf{1}\ \ \pm\imath\mathbf{1}\,)\,\Phi^E\ ,$$

one has $\Pi([\Phi^E]_\sim) = \phi_-^E\,(\phi_+^E)^{-1}$. Furthermore the following identities can be checked using the fact that Φ^E is Lagrangian:

$$(\phi_+^E)^*\,\phi_+^E\ =\ (\phi_-^E)^*\,\phi_-^E\ =\ (\Phi^E)^*\,\Phi^E\ ,\qquad (\phi_\pm^E)^*\partial_E\phi_\pm^E\ =\ (\Phi^E)^*\partial_E\Phi^E\ \pm\ \imath\,(\Phi^E)^*\mathcal{J}\partial_E\Phi^E\ . \tag{26}$$

Corresponding to the two terms in

$$\partial_E\,\Pi([\Phi^E]_\sim)\ =\ (\partial_E\phi_-^E)\,(\phi_+^E)^{-1}\ -\ \phi_-^E\,(\phi_+^E)^{-1}(\partial_E\phi_+^E)\,(\phi_+^E)^{-1}\ ,$$

there are two contributions C_1 and C_2 in (25). For the first one, it follows from cyclicity

$$C_1\ =\ \mathrm{Tr}\Big(\ \big((\phi_+^E)^*\phi_+^E\big)^{-1}\,(\phi_-^E)^*\,\partial_E\,\phi_-^E\ \Big)\ ,$$

while for the second

$$C_2\ =\ -\,\mathrm{Tr}\Big(\ (\phi_+^E)^{-1}\,\partial_E\,\phi_+^E\ \Big)\ =\ -\,\mathrm{Tr}\Big(\ \big((\phi_+^E)^*\phi_+^E\big)^{-1}\,(\phi_+^E)^*\,\partial_E\,\phi_+^E\ \Big)\ .$$

Combining them and appealing to (26) concludes the proof. □

Next let us calculate the pairing for two examples. The first one was already given by Arnold [Arn1]. For $\eta \in [0,\pi]$, introduce the symplectic matrices

$$R_\eta\ =\ \begin{pmatrix}\cos(\eta)\,\mathbf{1} & \sin(\eta)\,\mathbf{1}\\ -\sin(\eta)\,\mathbf{1} & \cos(\eta)\,\mathbf{1}\end{pmatrix}\ ,\qquad \mathcal{C}\,R_\eta\,\mathcal{C}^*\ =\ \begin{pmatrix}e^{\imath\eta}\,\mathbf{1} & \mathbf{0}\\ \mathbf{0} & e^{-\imath\eta}\,\mathbf{1}\end{pmatrix}\ ,$$

as well as the closed path $\Gamma = (R_\eta[\Phi]_\sim)_{\eta\in[0,\pi)}$ for an arbitrary $[\Phi]_\sim \in \mathbb{L}_L^{\mathbb{C}}$. As $\det(\Pi([R_\eta\Phi]_\sim)) = e^{2\imath L\eta}\det(\Pi([\Phi]_\sim))$, one deduces $\langle\,\omega\,|\,\Gamma\,\rangle = L$. The second example concerns transfer matrices.

Lemma 5 *Let $\mathcal{T}^E$ be a matrix built as in (2) from a selfadjoint matrix V and positive matrix T. For an arbitrary $[\Phi]_\sim \in \mathbb{L}_L^{\mathbb{C}}$ with $(\mathbf{1}\,\mathbf{0})\,\Phi$ invertible and $\mathcal{M} \in \mathrm{SP}(2L,\mathbb{C})$, consider the path $\Gamma = (\mathcal{M}\mathcal{T}^E[\Phi]_\sim)_{E\in\overline{\mathbb{R}}}$ where $\overline{\mathbb{R}} = \mathbb{R}\cup\{\infty\}$ is the one-point compactification. Then Γ is closed and $\langle\,\omega\,|\,\Gamma\,\rangle = L$. Moreover, $E\in\mathbb{R}\mapsto\int_\Gamma^E\omega$ is strictly monotonously increasing.*

Proof. First suppose that $\mathcal{M}=\mathbf{1}$. Then note that $\Pi([\mathcal{T}^E\Phi]_\sim) = \mathbf{1}+\mathcal{O}(E^{-1})$, hence the path is closed. Next one calculates

$$\mathcal{C}\,\mathcal{T}^E\,\mathcal{C}^* \;=\; \frac{1}{2}\begin{pmatrix} (E\,\mathbf{1}\,-\,V)\,T^{-1}-\imath(T+T^{-1}) & (E\,\mathbf{1}\,-\,V)\,T^{-1}+\imath(T-T^{-1}) \\ (E\,\mathbf{1}\,-\,V)\,T^{-1}-\imath(T-T^{-1}) & (E\,\mathbf{1}\,-\,V)\,T^{-1}+\imath(T+T^{-1}) \end{pmatrix}\,.$$

Let A^E and D^E denote the upper left and lower right entry. Then $\Im m\;\partial_E\,\log(\det(A^E))$ is equal to

$$\mathrm{Tr}\,\Big(\big(T^{-1}(E-V)^2T^{-1}+(T+T^{-1})^2+\imath(T^{-1}VT-TVT^{-1})\big)^{-1}(\mathbf{1}+T^{-2})\Big)\;.$$

As there is a similar expression for $\Im m\;\partial_E\,\log(\det(D^E))$, this shows that the integral in (23) is finite. In order to calculate the winding number, it is convenient to consider the homotopy

$$\mathcal{T}^E(\lambda)\;=\;\begin{pmatrix} (E\,\mathbf{1}\,-\,V(\lambda))\,T(\lambda)^{-1} & -T(\lambda) \\ T(\lambda)^{-1} & \mathbf{0}\end{pmatrix}\,,\qquad 0\leq\lambda\leq 1\,.$$

where $V(\lambda)=\lambda V$ and $T(\lambda)=\lambda T+(1-\lambda)\mathbf{1}$ (the latter is always positive). Then the pairing of $\Gamma(\lambda)=(\mathcal{T}^E(\lambda)[\Phi]_\sim)_{E\in\overline{\mathbb{R}}}$ with ω is independent of λ. Hence it is sufficient to calculate the pairing at $\lambda=0$, which is due to the above replaced into (23) given by

$$\langle\,\omega\,|\,\Gamma(0)\,\rangle\;=\;\int_{-\infty}^{\infty}\frac{dE}{\pi}\,\mathrm{Tr}\big((E^2+4)^{-1}\,2\,\mathbf{1}\big)\;=\;L\,,$$

completing the proof in the case $\mathcal{M}=\mathbf{1}$. If $\mathcal{M}\neq\mathbf{1}$, the winding number is the same because $\mathrm{SP}(2L,\mathbb{C})$ is arc-wise connected, as already pointed out above. The monotonicity can be checked using the r.h.s. of (24) for $\Phi^E=\mathcal{M}\mathcal{T}^E\Phi$. In fact, $(\Phi^E)^*\Phi^E$ is strictly positive, and

$$(\Phi^E)^*\mathcal{J}\partial_E\Phi^E\;=\;\Phi^*\begin{pmatrix} T^{-2} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}\Phi\,,$$

which is strictly positive by hypothesis. As the trace of a product of two positive operators is still positive, this concludes the proof. $\Box$

3 Jacobi matrices with matrix entries

Given integers $L, N \in \mathbb{N}$, let $(T_n)_{n=2,\ldots,N}$ and $(V_n)_{n=1,\ldots,N}$ be sequences of respectively positive and selfadjoint $L \times L$ matrices with complex entries. Furthermore let the left and right boundary conditions ζ and ξ be also self-adjoint $L \times L$ matrices. In the real and quaternion case, one chooses ζ and ξ symmetric and self-dual. Then the associated Jacobi matrix with matrix entries H^N_ξ is by definition the symmetric operator acting on states $\phi = (\phi_n)_{n=1,\ldots,N} \in \ell^2(1,\ldots,N) \otimes \mathbb{C}^L$ by

$$(H^N_\xi \phi)_n \;=\; T_{n+1}\phi_{n+1} + V_n\phi_n + T_n\phi_{n-1} \,, \qquad n = 1,\ldots,N \,, \tag{27}$$

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

$$\phi_0 \;=\; \zeta\,\phi_1 \,, \qquad \phi_{N+1} \;=\; \xi\,\phi_N \,. \tag{28}$$

One can also rewrite H^N_ξ defined in (27) and (28) more explicitly as a block diagonal matrix; this gives (1) albeit with V_1 and V_N replaced by $V_1 - \zeta$ and $V_N - \xi$. The dependence on ζ is not specified, but it could potentially be used for averaging purposes. If $\zeta = \xi = \mathbf{0}$ one speaks of Dirichlet boundary conditions.

3.1 Transfer matrices and dynamics of Lagrangian planes

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

$$H^N_\xi \phi \;=\; E\,\phi \,, \tag{29}$$

for a complex energy E in terms of the $2L \times 2L$ transfer matrices $\mathcal{T}^E_n$ defined in (2). For a real energy $E \in \mathbb{R}$, each transfer matrix is in the symplectic group $\mathrm{SP}(2L,\mathbb{C})$. If H^N is, moreover, real or self-dual, then the transfer matrices are in the subgroups $\mathrm{SP}(2L,\mathbb{R})$ and $\mathrm{SP}(2L,\mathbb{H})$ respectively. The Schrödinger equation (29) is satisfied if and only if

$$\begin{pmatrix} T_{n+1}\phi_{n+1} \\ \phi_n \end{pmatrix} \;=\; \mathcal{T}^E_n \begin{pmatrix} T_n\phi_n \\ \phi_{n-1} \end{pmatrix} \,, \qquad n = 1,\ldots,N \,,$$

and the boundary conditions (28) hold, namely

$$\begin{pmatrix} T_1\phi_1 \\ \phi_0 \end{pmatrix} \;\in\; \Phi_\zeta\,\mathbb{C}^L \,, \qquad \begin{pmatrix} T_{N+1}\phi_{N+1} \\ \phi_N \end{pmatrix} \;\in\; \Psi_\xi\,\mathbb{C}^L \,, \tag{30}$$

where we introduced for later convenience the notations

$$\Phi_\zeta \;=\; \begin{pmatrix} \mathbf{1} \\ \zeta \end{pmatrix} \,, \qquad \Psi_\xi \;=\; \begin{pmatrix} \xi \\ \mathbf{1} \end{pmatrix}$$

Both of the two L-dimensional subspaces of $\mathbb{C}^{2L}$ appearing in the conditions (30) are Lagrangian. One way to search for eigenvalues is to consider the whole subspace in the left equation of (30), then to follow its evolution under application of the transfer matrices, and finally to check whether at N the resulting subspace has a non-trivial intersection with the subspace on the r.h.s. of (30). For perturbation theory in Section 4, it is useful to incorporate a symplectic basis change $\mathcal{M} \in \mathrm{SP}(2L,\mathbb{C})$ which can be conveniently chosen later on. In the one-dimensional situation this corresponds to pass to modified Prüfer variables. If H^N is real or self-dual, one chooses $\mathcal{M} \in \mathrm{SP}(2L,\mathbb{R})$ or $\mathcal{M} \in \mathrm{SP}(2L,\mathbb{H})$. As above, half-dimensional subspaces will be described by $2L \times L$ matrices Φ^E_n of rank L composed of column vectors spanning it. Then their dynamics under application of the $\mathcal{M}$-transformed transfer matrices is

$$\Phi^E_n \;=\; \mathcal{M}\,\mathcal{T}^E_n\,\mathcal{M}^{-1}\,\Phi^E_{n-1}\;, \qquad \Phi^E_0 \;=\; \mathcal{M}\,\Phi_\zeta\;. \tag{31}$$

If $E \in \mathbb{R}$, these planes are Lagrangian. As the boundary condition on the left boundary is satisfied automatically (it is chosen as the initial condition), the second condition in (30) multiplied by $\mathcal{M}$ together with the Wronski test (17) leads to

$$\text{multiplicity of } E \text{ as eigenvalue of } H^N_\xi \;=\; L \;-\; \mathrm{rank}\left((\mathcal{M}\,\Psi_\xi)^*\;\mathcal{J}\;\Phi^E_N\right)\;. \tag{32}$$

This implies also

Proposition 5 *Let* $\Gamma = ([\Phi^E_N]_\sim)_{E\in\overline{\mathbb{R}}}$. *For every* $\xi \in \mathrm{Sym}(L,\mathbb{R}) \cap \mathrm{Self}(L,\mathbb{C})$, *the set* $\{E \in \overline{\mathbb{R}} \mid \Gamma(E) \in \mathbb{L}^{\mathbb{C},\xi}_L\}$ *of intersections with the singular cycle* $\mathbb{L}^{\mathbb{C},\xi}_L$ *is finite.*

The dynamics (31) is more easily controlled under the stereographic projection. Let us first consider the case $\Im m(E) > 0$. In this situation the stereographic projection π of (31) gives a dynamics in the upper half-plane $\mathbb{U}^{\mathbb{C}}_L$, or $\mathbb{U}^{\mathbb{R}}_L$ if H^N is real and $\mathbb{U}^{\mathbb{H}}_L$ if H^N is self-dual. In fact, $Z^E_1 = \pi(\Phi^E_1) = \mathcal{M}\cdot(E\,\mathbf{1} - V_1 - \zeta)$ is in $\mathbb{U}^{\mathbb{C}}_L$ and, moreover, the transfer matrices factor as follows:

$$\mathcal{T}^E_n \;=\; \begin{pmatrix} \mathbf{1} & \imath\,\Im m(E)\,\mathbf{1} \\ \mathbf{0} & \mathbf{1} \end{pmatrix} \begin{pmatrix} (\Re e(E)\,\mathbf{1} \,-\, V_n)\,T_n^{-1} & -T_n \\ T_n^{-1} & \mathbf{0} \end{pmatrix}\;.$$

The matrix on the right is in the symplectic group $\mathrm{SP}(2L,\mathbb{C})$ acting on $\mathbb{U}^{\mathbb{C}}_L$, the one on the left also sends $\mathbb{U}^{\mathbb{C}}_L$ to $\mathbb{U}^{\mathbb{C}}_L$ because of (16). The same applies for real and self-dual H^N. Hence the following Möbius action is well-defined:

$$Z^E_n \;=\; \mathcal{M}\,\mathcal{T}^E_n\,\mathcal{M}^{-1}\cdot Z^E_{n-1}\;, \qquad Z^E_1 \;=\; \mathcal{M}\cdot(E\,\mathbf{1} \,-\, V_1 \,-\, \zeta)\;, \tag{33}$$

In the case $\mathcal{M} = \mathbf{1}$, this is a matricial Ricatti equation $Z^E_n = E - V_n + T_n(Z^E_{n-1})^{-1}T_n$. Comparing with (31),

$$Z^E_n \;=\; \pi([\Phi^E_n]_\sim)\;, \qquad n = 1,\ldots,N\;.$$

In particular, $[\Phi_n^E]_\sim$ is in the domain $\mathbb{G}_L^{\rm inv}$ of π whenever $\Im m(E) > 0$. If the boundary condition ζ is invertible, one may also set $Z_0^E = \mathcal{M}\cdot\zeta^{-1}$ and then $Z_1^E = \mathcal{M}\mathcal{T}_1^E\mathcal{M}^{-1}\cdot Z_0^E$, even though Z_0^E is not in $\mathbb{U}_L^{\mathbb{C}}$. Furthermore, the map $E\in\mathbb{U}_1^{\mathbb{C}} \mapsto Z_N^E \in \mathbb{U}_L^{\mathbb{C}}$ is analytic (Herglotz). The map has poles on the real axis as can be read off the Dean-Martin identity (46) proven below, but will not be used in the sequel.

As real energies are not always permitted, the Z_n^E are not convenient for the calculation of the eigenvalues. For any E with $\Im m(E)\geq 0$, let us rather use

$$U_n^E \;=\; \Pi([\Phi_n^E]_\sim)\;, \qquad n=0,\ldots,N\;.$$

For real E, this is well-defined and U_n^E is a unitary because of Theorem 4. This unitary is symmetric or self-dual if H^N is real or self-dual. Iterating (31) and recalling the definition of the stereographic projection shows that U_n^E is actually of the explicit form given in (3) if one chooses $\mathcal{M}=\mathbf{1}$. Hence this proves Theorem 1(i) and part of (ii). For $\Im m(E)>0$, the above arguments imply Z_n^E is well-defined and hence also $U_n^E = \mathcal{C}\cdot Z_n^E$. One, moreover, concludes that $U_n^E=\mathcal{C}\cdot Z_n^E$ is in the generalized unit disc $\mathbb{D}_L^{\mathbb{C}}$ (for $n\neq 0$). The dynamics is given by

$$U_n^E \;=\; \mathcal{C}\,\mathcal{M}\,\mathcal{T}_n^E\,\mathcal{M}^{-1}\,\mathcal{C}^*\cdot U_{n-1}^E\;, \qquad U_0^E \;=\mathcal{M}\cdot(\mathbf{1}\,-\,\imath\,\zeta)\,(\mathbf{1}\,+\,\imath\,\zeta)^{-1}\;. \tag{34}$$

For $\Im m(E)>0$, this is just the Cayley transform of (33), while for $E\in\mathbb{R}$, it is the dynamics of Theorem 5. The following lemma proves Theorem 1(ii) and the first part of (iii).

Lemma 6 *The map $E\mapsto U_N^E$ is analytic in a neighborhood of $\overline{\mathbb{U}_1^{\mathbb{C}}} = \mathbb{U}_1^{\mathbb{C}}\cup\partial\mathbb{U}_1^{\mathbb{C}}$. At level crossings, the eigenvalues and eigenvectors can be enumerated such that they are analytic in a neighborhood of $\overline{\mathbb{U}_1^{\mathbb{C}}}$ as well.*

Proof. Analyticity of U_N^E away from the real axis follows from the analyticity of Z_N^E because $U_n^E=\mathcal{C}\cdot Z_n^E$ and the inverse in the Möbius transformation is also well-defined, *cf.* Section 2.4. Moreover, the characteristic polynomial is a Weierstrass polynomial that has a global Puiseux expansion which is analytic in the Lth root of E. Hence the eigenvalues and eigenvectors can be chosen (at level crossings) such that they are analytic in the Lth root of E (*e.g.* [Kat, Chapter II]). It will follow from the arguments below that the Puiseux expansion actually reduces to a power series expansion in E.

Now we analyze in more detail the situation in a neighborhood of the real axis. The plane Φ_N^E is a polynomial in E. Let us use the notations $\Phi_N^E = \begin{pmatrix} a^E \\ b^E\end{pmatrix}$. It follows from the argument in (10) that $a^E+\imath\,b^E$ has maximal rank for $E\in\mathbb{R}$ so that $E\in\mathbb{R}\mapsto\det(a^E+\imath\,b^E)$ has no zero. Moreover, one has the large E asymptotics

$$\Phi_N^E \;=\; E^{NL}\,\mathcal{M}\,\begin{pmatrix} \prod_{n=1}^N T_n^{-1} \\ \mathbf{0}\end{pmatrix} \;+\; \mathcal{O}(E^{NL-1})\;. \tag{35}$$

which implies

$$\det(a^E + \imath\, b^E) \;=\; E^{NL}\,\det\left(\begin{pmatrix}\mathbf{1}\\ \imath\,\mathbf{1}\end{pmatrix}^t \mathcal{M}\begin{pmatrix}\mathbf{1}\\ \mathbf{0}\end{pmatrix}\right)\prod_{n=1}^{N}\det(T_n)^{-1} \;+\; \mathcal{O}(E^{NL-1})\;.$$

Therefore $\inf_{E\in\mathbb{R}}|\det(a^E+\imath\, b^E)|>0$ and the infimum is realized at some finite E. A perturbative argument shows that also $\inf_{E\in S_\delta}|\det(a^E+\imath\, b^E)|>0$ where $S_\delta=\{E\in\mathbb{C}\,|\,|\Im m(E)|<\delta\}$ is a strip of some width $\delta>0$. Calculating the inverse with the Laplace formula shows that $(a^E+\imath\, b^E)^{-1}$ is also analytic in S_δ. Thus also $U_N^E=(a^E-\imath\, b^E)(a^E+\imath\, b^E)^{-1}$ is analytic in S_δ and thus analytic in a neighborhood of $\overline{\mathbb{U}_1^{\mathbb{C}}}$ due to the above.

Finally one can appeal to degenerate perturbation theory [Kat, Theorem II.1.10] in order to deduce that the eigenvalues and eigenvectors of the unitary matrix U_N^E (hence E real) are also analytic in a neighborhood of the real axis, that is are given by an analytic Puiseux expansion. As this neighborhood has an open intersection with the upper half-plane, the above Puiseux expansion is therefore also analytic, namely only contains powers of E. $\square$

It follows from (35) that

$$U_N^E \;=\; \mathcal{C}\,\mathcal{M}\,\mathcal{C}^*\cdot\mathbf{1} \;+\; \mathcal{O}(E^{-1})\;. \tag{36}$$

Let $0\leq\theta_l^{\mathcal{M}}<2\pi$ be the eigenphases of the symmetric unitary $\mathcal{C}\mathcal{M}\mathcal{C}^*\cdot\mathbf{1}$. The eigenvalues of U_N^E, chosen to be real analytic in $E\in\mathbb{R}$ as in Lemma 6, are denoted by $e^{\imath\theta_{N,l}^E}$, $l=1,\ldots,L$. The eigenphases are chosen such that $\theta_{N,l}^E\to\theta_l^{\mathcal{M}}$ for $E\to-\infty$. In the case $\mathcal{M}=\mathbf{1}$, one hence has $\theta_{N,l}^E\to 0$ for $E\to-\infty$ as in Theorem 1.

Let us conclude this section by choosing particular right boundary conditions, namely, for $\varphi\in(0,2\pi)$,

$$\xi \;=\; -\cot(\tfrac{\varphi}{2})\,\mathcal{M}^{-1}\cdot\mathbf{1} \qquad\Longrightarrow\qquad \big[\mathcal{M}\Psi_\xi\big]_\sim \;=\; \big[\Psi_{-\cot(\frac{\varphi}{2})\,\mathbf{1}}\big]_\sim\;.$$

The corresponding Hamiltonian will be denoted by H_φ^N. If $\mathcal{M}=\mathbf{1}$ and $\varphi=\pi$, these are Dirichlet boundary conditions on the right boundary. Due to Proposition 3 and (18), the eigenvalue condition (32) becomes

$$\text{multiplicity of } E \text{ as eigenvalue of } H_\varphi^N \;=\; \text{multiplicity of } e^{\imath\varphi} \text{ as eigenvalue of } U_N^E\;. \tag{37}$$

Setting $\mathcal{M}=\mathbf{1}$ and $\varphi=\pi$, this proves Theorem 1(iv).

3.2 Monotonicity and transversality

This section provides the proof of Theorem 1(v) (just set $\mathcal{M} = \mathbf{1}$ in the below). Of course, the second statement of Theorem 1(v) follows immediately from the first one upon evaluation in the eigenspaces of U_N^E. The following proposition also shows that the curve $\Gamma = ([\Phi_N^E]_\sim)_{E\in\overline{\mathbb{R}}}$ is transversal to the singular cycle $\mathbb{L}_L^\varphi$ and always crosses it from the negative to the positive side.

Proposition 6 *For $E \in \mathbb{R}$ and $N \geq 2$, one has*

$$\frac{1}{\imath}\,(U_N^E)^*\,\partial_E\,U_N^E \;>\; 0\;.$$

Proof. As in the proof of Lemma 4, let us introduce $\phi_\pm^E = (\,\mathbf{1}\;\;\pm\imath\mathbf{1}\,)\;\Phi_N^E$. These are invertible $L\times L$ matrices and one has $U_N^E = \phi_-^E(\phi_+^E)^{-1} = ((\phi_-^E)^{-1})^*(\phi_+^E)^*$. Now

$$(U_N^E)^*\,\partial_E\,U_N^E \;=\; ((\phi_+^E)^{-1})^*\Big[\,(\phi_-^E)^*\partial_E\phi_-^E\;-\;(\phi_+^E)^*\partial_E\phi_+^E\Big](\phi_+^E)^{-1}\;.$$

Thus it is sufficient to verify positive definiteness of

$$\frac{1}{\imath}\,\Big[\,(\phi_-^E)^*\partial_E\phi_-^E\;-\;(\phi_+^E)^*\partial_E\phi_+^E\Big]\;=\;2\,(\Phi_N^E)^*\,\mathcal{J}\,\partial_E\Phi_N^E\;.$$

¿From the product rule follows that

$$\partial_E\Phi_N^E\;=\;\sum_{n=1}^N\,\mathcal{M}\left(\prod_{l=n+1}^N\,\mathcal{T}_l^E\right)\,\left(\partial_E\mathcal{T}_n^E\right)\,\left(\prod_{l=1}^{n-1}\,\mathcal{T}_l^E\right)\,\Phi_\zeta\;.$$

Using $\mathcal{M}^*\mathcal{J}\mathcal{M} = \mathcal{J}$, this implies that

$$(\Phi_N^E)^*\,\mathcal{J}\,\partial_E\Phi_N^E\;=\;\sum_{n=1}^N\,\Phi_\zeta^*\,\left(\prod_{l=1}^{n-1}\,\mathcal{T}_l^E\right)^*\,\left(\mathcal{T}_n^E\right)^*\,\mathcal{J}\,\left(\partial_E\mathcal{T}_n^E\right)\,\left(\prod_{l=1}^{n-1}\,\mathcal{T}_l^E\right)\,\Phi_\zeta\;. \tag{38}$$

As one checks that

$$\left(\mathcal{T}_n^E\right)^*\,\mathcal{J}\,\left(\partial_E\mathcal{T}_n^E\right)\;=\;\begin{pmatrix}(T_nT_n^*)^{-1} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}\;,$$

each of the summands in (38) is positive semi-definite. In order to prove the strict inequality, it is sufficient that the first two terms $n = 1, 2$ in (38) give a strictly positive contribution. Hence let us verify that

$$\left(\mathcal{T}_2^E\right)^*\,\begin{pmatrix}(T_1T_1^*)^{-1} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}\,\mathcal{T}_2^E\;+\;\begin{pmatrix}(T_2T_2^*)^{-1} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}\;>\;0\;.$$

For this purpose let us show that the kernel of the matrix on the l.h.s. is empty. As $\left((\mathcal{T}_2^E)^*\right)^{-1} = -\mathcal{J}\mathcal{T}_2^E\mathcal{J}$, we thus have to show that a vector $\begin{pmatrix} v \\ w \end{pmatrix} \in \mathbb{C}^{2L}$ satisfying

$$\mathcal{J}\begin{pmatrix} (T_1T_1^*)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \mathcal{T}_2^E \begin{pmatrix} v \\ w \end{pmatrix} = \mathcal{T}_2^E\,\mathcal{J}\begin{pmatrix} (T_2T_2^*)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}\begin{pmatrix} v \\ w \end{pmatrix},$$

actually vanishes. Carrying out the matrix multiplications, one readily checks that this is the case. □

Of course, one can regroup the terms in (38) into packages of two successive contributions and each of them is positive by the same argument. If this bound is uniform for the packages (*e.g.* the spectrum of the T_n is uniformly bounded away from 0), one actually deduces an improved lower bound by $C_E N$ for some $C_E > 0$.

3.3 The total rotation number

In this section, we complete the proof of Theorem 1, in particular the second part of item (iii). Throughout $E \in \mathbb{R}$. The total rotation number is defined by

$$\Theta_N^E = \int_{-\infty}^{E} de\; \Im m\; \partial_e\; \log(\det(U_N^e))\,. \tag{39}$$

It will be shown shortly that the integral converges. Using the notations of Section 2.8, $\Theta_N^E = \int_\Gamma^E \omega$ for $\Gamma = ([\Phi_N^E]_\sim)_{E\in\overline{\mathbb{R}}}$. Let $\theta_{N,l}^E$ be the analytic eigenphases of U_N^E as introduced after (36). We deduce after integration of (39) that

$$\Theta_N^E = \sum_{l=1}^{L}\left(\theta_{N,l}^E - \theta_l^{\mathcal{M}}\right). \tag{40}$$

This justifies the term *total rotation number*. The following result could also be deduced from the results of the previous section, but its proof (a homotopy argument) directly completes the proof of Theorem 1(iii).

Proposition 7 *The total rotation number Θ_N^E is well-defined and satisfies*

$$\lim_{E\to-\infty}\Theta_N^E = 0\,, \qquad \lim_{E\to\infty}\Theta_N^E = 2\pi\,N\,L\,.$$

Proof. Expanding $\Phi^E_N = \mathcal{M}\prod_{n=1}^N \mathcal{T}^E_n \,\Phi_\zeta$ shows

$$\begin{aligned}\big((\Phi^E_N)^*\Phi^E_N\big)^{-1} \;&=\; \left(\Phi^*_\zeta\, E^{2N}\begin{pmatrix}\mathbf{1} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}^N \mathcal{M}^*\mathcal{M}\begin{pmatrix}\mathbf{1} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}^N \Phi_\zeta \;+\; \mathcal{O}(E^{2N-1})\right)^{-1}\\ &=\; E^{-2N}\begin{pmatrix}\mathbf{1}\\ \mathbf{0}\end{pmatrix}^* \mathcal{M}^*\mathcal{M}\begin{pmatrix}\mathbf{1}\\ \mathbf{0}\end{pmatrix} \;+\; \mathcal{O}(E^{-2N-1})\,.\end{aligned}$$

Similarly one verifies

$$(\Phi^E_N)^*\,\mathcal{J}\,\partial_E\Phi^E_N \;=\; \mathcal{O}(E^{2N-2})\,.$$

Hence follows

$$\big((\Phi^E_N)^*\Phi^E_N\big)^{-1}\,(\Phi^E_N)^*\,\mathcal{J}\,\partial_E\Phi^E_N \;=\; \mathcal{O}(E^{-2})\,,$$

so that the integral in (39) exists due to (24), which can alternatively be derived from Lemma 5. Furthermore, one deduces from (36) that $\Gamma = ([\Phi^E_N]_\sim)_{E\in\overline{\mathbb{R}}}$ is a closed path in $\mathbb{L}^{\mathbb{C}}_L$ and its winding number is given by

$$\langle\,\omega\,|\,\Gamma\,\rangle \;=\; \frac{1}{2\pi}\lim_{E\to\infty}\,\Theta^E_N\,.$$

In order to calculate the winding number and prove the last statement of the proposition, one applies Proposition 4 and Lemma 5 iteratively to the path $\Gamma = ([\mathcal{M}\prod_{n=1}^N \mathcal{T}^E_n\Phi_\zeta]_\sim)_{E\in\overline{\mathbb{R}}}$. Alternatively one can use a homotopy $H^N(\lambda)$ from $H^N(1) = H^N_\varphi$ to $H^N(0)$ which is the sum of L un-coupled one-dimensional discrete Laplacians (using the homotopy of the proof of Lemma 5 on every site n). For each of the one-dimensional discrete Laplacians the winding number is again easy to calculate and equal to N. $\Box$

Proof of the last statement of Theorem 1(iii). The homotopy discussed at the end of the proof of Proposition 7 is analytic and hence one deduces $\theta^E_{N,l} - \theta^{\mathcal{M}}_l \to 2\pi N$ for $E\to\infty$ for each l as this is the case for the one-dimensional discrete Laplacian. $\Box$

Remark Using Proposition 7 one can also give a nice alternative proof of $\partial_E\theta^E_{N,l}\geq 0$. Indeed, according to (37), the unitary U^E_N can be used in order to calculate the spectrum of H^N_φ for every $\varphi\in(0,2\pi)$. Counting multiplicities, this spectrum consists of NL eigenvalues. By Proposition 7 and Theorem 6, the total number of passages of eigenvalues $\theta^E_{N,l}$ by φ (intersections with the singular cycle $\mathbb{L}^\varphi_L$) is bounded below by NL. As there cannot be more than NL, all these passages have to be in the positive sense because a passage in the negative sense would lead to at least two more eigenvalues of H^N_φ.

3.4 Telescoping the total rotation number

By the results of the last section and due to the fact that a change of right boundary condition can change the number of eigenvalues by at most L, one has

$$\left| \frac{1}{2\pi} \Theta_N^E - \#\left\{ \text{ eigenvalues of } H_\xi^N \leq E \right\} \right| \leq 2L . \tag{41}$$

Hence Θ_N^E allows to count the eigenvalues of H^N up to boundary terms. For this purpose it is useful to telescope Θ_N^E into N contributions stemming from the L-dimensional slices:

$$\Theta_N^E = \sum_{n=1}^N \int_{-\infty}^E de\ \Im m\ \partial_e \log\left(\frac{\det(U_n^e)}{\det(U_{n-1}^e)}\right) .$$

Here we have used (34) and the fact that U_0^e is independent of e. This is indeed a good way to telescope because $U_n^e = \mathcal{C}\,\mathcal{M}\,\mathcal{T}_n^e\,\mathcal{M}^{-1}\,\mathcal{C}^* \cdot U_{n-1}^e$ so that Proposition 4 and Lemma 5 imply that each summand satisfies

$$\left| \int_{-\infty}^E de\ \Im m\ \partial_e \log\left(\frac{\det(\mathcal{C}\,\mathcal{M}\,\mathcal{T}_n^e\,\mathcal{M}^{-1}\,\mathcal{C}^* \cdot U_{n-1}^e)}{\det(U_{n-1}^e)}\right) \right| \leq 2L .$$

Moreover, with the notation

$$\mathcal{C}\,\mathcal{M}\,\mathcal{T}_n^E\,\mathcal{M}^{-1}\,\mathcal{C}^* = \begin{pmatrix} A_n^E & B_n^E \\ C_n^E & D_n^E \end{pmatrix} , \tag{42}$$

the same calculation as in Proposition 4 implies that

$$\Theta_N^E = \sum_{n=1}^N \int_{-\infty}^E de\ \Im m\ \partial_e \log\Big(\det\big((A_n^e + B_n^e\,(U_{n-1}^e)^*)(D_n^e + C_n^e\,U_{n-1}^e)^{-1} \big) \Big) . \tag{43}$$

Now it is actually possible to apply the fundamental theorem in every summand by determining the branch of the logarithm uniquely from the transfer matrix $\mathcal{T}_n^E$, and independent of the prior transfer matrices. Indeed, one can factor out $\det(A_n^e(D_n^e)^{-1})$ and use the fact that $(A_n^e)^{-1}B_n^e$ and $(D_n^e)^{-1}C_n^e$ have norm less than 1 by Lemma 2, so that as in the proof of Proposition 4:

$$\begin{aligned}\Theta_N^E = \sum_{n=1}^N \Im m\ \Big[& \int_{-\infty}^E de\ \partial_e \log\big(\det(A_n^e(D_n^e)^{-1})\big) \\ & + \mathrm{Tr}\big(\log\big(\mathbf{1} + (A_n^E)^{-1}\,B_n^E\,(U_{n-1}^E)^*\big)\big) - \mathrm{Tr}\big(\log\big(\mathbf{1} + (D_n^E)^{-1}\,C_n^E\,U_{n-1}^E\big)\big)\Big] .\end{aligned} \tag{44}$$

A refined version of this formula is exploited in Section 4.

3.5 The Dean-Martin identity

In this and the next two sections, $\mathcal{M} = \mathbf{1}$ and $\xi = \mathbf{0}$ (Dirichlet boundary conditions on the right boundary). The Hamiltonian will be denoted by H^N without a further index. According to (32), E is an eigenvalue of H^N if and only if

$$\det\left(\begin{pmatrix}\mathbf{0} & \mathbf{1}\end{pmatrix} \mathcal{J}\, \Phi_N^E\right) \;=\; \det\left(\begin{pmatrix}\mathbf{1}\, \mathbf{0}\end{pmatrix} \prod_{n=1}^{N} \mathcal{T}_n^E\, \Phi_\zeta\right) \;=\; 0\,.$$

Due to (32), the multiplicity of the zero is the multiplicity of the eigenvalue. Therefore the l.h.s. of this equation is a polynomial of degree NL in E with zeros exactly at the NL eigenvalues of H^N. Comparing the leading order coefficient, one deduces a formula for the characteristic polynomial:

$$\det(E\,\mathbf{1} - H^N) \;=\; \det\left(\begin{pmatrix}\mathbf{1}\, \mathbf{0}\end{pmatrix} \Phi_N^E\right) \prod_{n=1}^{N} \det(T_n^{-1})\,. \tag{45}$$

In order to find a recurrence relation for the characteristic polynomials, let us suppose that $\Im m(E) > 0$ and note that $Z_N^E = \begin{pmatrix}\mathbf{1} & \mathbf{0}\end{pmatrix} \Phi_N^E \left(\begin{pmatrix}\mathbf{1}\, \mathbf{0}\end{pmatrix} \Phi_{N-1}^E\right)^{-1} T_N$. Taking the determinant of this formula, the identity (45) applied twice gives

$$\det(Z_N^E) \;=\; \frac{\det\big(E\,\mathbf{1} - H^N\big)}{\det\big(E\,\mathbf{1} - H^{N-1}\big)}\,. \tag{46}$$

Let us call this the Dean-Martin identity, due to the contribution [DM]. These authors then used the identity (46) at real energies in order to calculate the spectrum of H_π^{N-1} by counting the singularities of $\det(Z_N^E)$. This can be made more explicit by adding a small imaginary part $\delta > 0$ to the energy. Then consider the path $E \in \mathbb{R} \mapsto \det(Z_N^{E+\imath\delta}) \in \mathbb{C}$. Even though $Z_N^{E+\imath\delta}$ is in the upper half-plane, its determinant may well have a negative imaginary part. However, it never takes the values $\pm\,\imath$. Now each passage of the path (near) by an eigenvalue of H^{N-1} leads to an arc in either the upper or lower half-plane with passage by either $\imath/\delta$ or $-\imath/\delta$, pending on the sign of the numerator in (46). Both arcs turn out to be in the positive orientation. A multiple eigenvalue leads to a multiple arc. The topologically interesting quantity is the winding numbers of the path around $\imath$ and $-\imath$. Calculating the sum of the corresponding phase integrals gives a total rotation number which in the limit $\delta \to 0$ coincides with Θ_N^E. This allows to give a nice alternative, but considerably more complicated proof of Proposition 7. In the case $L = 1$, all the arcs are in the upper half-plane and the argument just sketched is particularly simple.

3.6 Green's function and continued fraction expansion

The aim of this short section is to illustrate the use of the dynamics in the upper half-plane. For $\Im m(E) > 0$, the $L \times L$ Green's matrix $G^{E,N}_{n,m}$ for $1 \leq n, m \leq N$ is defined by

$$G^{E,N}_{n,m}(k,l) \;=\; \langle n,k|\,(H^N - E\,\mathbf{1})^{-1}\,|m,l\rangle\;, \qquad k,l = 1,\ldots,L\;.$$

It follows from the Schur complement formula that

$$G^{E,N}_{N,N} \;=\; \Big(V_N - E\,\mathbf{1} - T_N G^{E,N-1}_{N-1,N-1} T_N\Big)^{-1}\;.$$

Iteration of this formula gives a matricial continued fraction expansion:

$$G^{E,N}_{N,N} \;=\; \bigg(V_N - E\,\mathbf{1} - T_N \Big(\cdots \big(V_2 - E\,\mathbf{1} - T_2(V_1 - E\,\mathbf{1} + \zeta)^{-1}T_2\big)^{-1}\cdots\Big)^{-1} T_N\bigg)^{-1}\;.$$

As $Z^E_1 = E\,\mathbf{1} - V_1 - \zeta$, one sees that this is just the iteration of the Ricatti equation. Hence one deduces

$$G^{E,N}_{N,N} \;=\; -\,(Z^E_N)^{-1} \;=\; -\,\pi(\Phi^E_N)^{-1}\;,$$

where the inverse $(Z^E_N)^{-1}$ exists because it is given by the Möbius transformation of $Z^E_N \in \mathbb{U}^{\mathbb{C}}_L$ with $\imath\,\mathcal{J} \in \mathrm{SP}(2L,\mathbb{C})$. Hence $G^{E,N}_{N,N} \in \mathbb{U}^{\mathbb{C}}_L$. Furthermore the geometric resolvent identity shows

$$G^{E,N}_{1,N} \;=\; -\,G^{E,N-1}_{1,N-1}\,T_N\,G^{E,N}_{N,N}\;.$$

These identities allow us to note a few useful identities linking the entries of the transfer matrix

$$\mathcal{T}^E_N \cdot \ldots \cdot \mathcal{T}^E_1 \;=\; \begin{pmatrix} A & B \\ C & D \end{pmatrix}\;,$$

to the Green's function:

$$A^{-1} \;=\; -\,G^{E,N}_{1,N}\;, \qquad C^{-1} \;=\; -\,G^{E,N-1}_{1,N-1}\,T_N\;, \qquad CA^{-1} \;=\; -\,G^{E,N}_{N,N}\;, \qquad A^{-1}B \;=\; G^{E,N}_{1,1}\;.$$

It is also possible to express B^{-1}, D^{-1}, DB^{-1} and $C^{-1}D$ in terms of Green's functions.

3.7 Eigenvalue interlacing

In this section, the above information on the spectrum of Jacobi matrices with matrix entries is complemented by a simple consequence of the min-max principle. In the case $L = 1$ of a Jacobi matrix, this is the theorem on alternation of zeros of the associated orthogonal polynomials. It also implies that the bottom (resp. top) of the spectrum of H^N is less (resp. larger) than or equal the bottom (resp. top) of the spectrum of H^{N-1}.

Proposition 8 *Let H^N and H^{N-1} be defined with Dirichlet boundary conditions on the right boundary. Then the eigenvalues of H^N and H^{N-1} satisfy the following interlacing property:*

$$E_j^N \;\leq\; E_j^{N-1} \;\leq\; E_{j+L}^N \;, \qquad j = 1, \ldots, (N-1)L \;.$$

Proof. Let $\mathcal{H}_N = \ell^2(1, \ldots, N) \otimes \mathbb{C}^L$ and Π_N the projection in $\mathcal{H}_N$ on the states on the right boundary, namely, in Dirac notation, on the span of $(|N, l\rangle)_{l=1,\ldots,L}$. Hence $\mathcal{H}_{N-1} \cong (\mathbf{1} - \Pi_N)\mathcal{H}_N$ and $\mathcal{H}_{N-1} \subset \mathcal{H}_N$ with the natural embedding. Also $H^{N-1}|\psi\rangle = H^N|\psi\rangle$ for $\psi \in \mathcal{H}_{N-1}$, *i.e.* $\Pi_N\psi = 0$ (the natural embedding is suppressed in this notation). The min-max principle states:

$$E_j^N \;=\; \sup_{U \subset \mathcal{H}_N \,,\, \dim(U) \leq j} \;\; \inf_{\psi \in U^\perp \,,\, \|\psi\|=1} \;\; \langle \psi \,|\, H^N \,|\, \psi \rangle \;,$$

where the supremum is over subspaces U of $\mathcal{H}_N$, and the infimum over unit vectors in their orthogonal complement. For H^{N-1}, the above facts imply

$$E_j^{N-1} \;=\; \sup_{U \subset \mathcal{H}_N \,,\, \dim(U) \leq j \,,\, \Pi_N U = 0} \;\; \inf_{\psi \in U^\perp \,,\, \|\psi\|=1 \,,\, \Pi_N\psi = 0} \;\; \langle \psi \,|\, H^N \,|\, \psi \rangle \;,$$

where the orthogonal complement is calculated in $\mathcal{H}_N$. Hence the inequality $E_j^{N-1} \geq E_j^N$ follows because the condition $\Pi_N U = 0$ is redundant and then one obtains a lower bound by dropping the constraint $\Pi_N\psi = 0$. Next, for a subspace $U \subset \mathcal{H}_N$ with $\Pi_N U = 0$, let $\tilde{U} = U \oplus \Pi_N\mathcal{H}_N$. Then $\dim(\tilde{U}) = \dim(U) + L$. Furthermore, the conditions $\psi \in U^\perp$ and $\Pi_N\psi = 0$ are equivalent to $\psi \in \tilde{U}^\perp$. Therefore, upon relaxing the constraints on the supremum:

$$E_j^{N-1} \;\geq\; \sup_{\tilde{U} \subset \mathcal{H}_N \,,\, \dim(\tilde{U}) \leq j+L} \;\; \inf_{\psi \in \tilde{U}^\perp \,,\, \|\psi\|=1} \;\; \langle \psi \,|\, H^N \,|\, \psi \rangle \;=\; E_{j+L}^N \;,$$

which is the second inequality. $\square$

4 Jacobi matrices with random matrix entries

In this section we consider Jacobi matrices $H^N(\omega)$ with matrix entries $\omega = (V_n, T_n)_{n \geq 1}$ which are independent and identically distributed random variables drawn from a bounded ensemble $(V_\sigma, T_\sigma)_{\sigma \in \Sigma}$ of symmetric and positive real matrices. Expectation w.r.t. to their distribution will be denoted by $\mathbf{E}_\sigma$ or simply by $\mathbf{E}$. All formulas in Section 4.1 also hold for more general covariant operator families and systems without time-reversal symmetry. Associated to each ω are transfer matrices $\mathcal{T}_n^E(\omega)$, Lagrangian planes $\Phi_n^E(\omega)$, their parametrizations $Z_n^E(\omega)$ and $U_n^E(\omega)$, matrix entries $A_n^E(\omega)$ and $B_n^E(\omega)$ as in (42), total rotations, etc. In order not to overload notation, the index ω is suppressed throughout. The basis change $\mathcal{M}$ will be taken independent of ω though.

4.1 Integrated density of states and sum of Lyapunov exponents

The integrated density of states of a random family of Jacobi matrices with matrix entries is defined by [CS, BL, CL]

$$\mathcal{N}(E) \;=\; \lim_{N\to\infty} \frac{1}{N\,L}\,\mathbf{E}\,\#\left\{\text{ eigenvalues of } H^N \;\leq\; E\right\}\;.$$

According to (41), (43) and the fact that $C_e = \overline{B_e}$ and $D_e = \overline{A_e}$, one has

$$\mathcal{N}(E) \;=\; \lim_{N\to\infty} \frac{1}{N\,L} \sum_{n=1}^{N} \int_{-\infty}^{E} \frac{de}{\pi}\, \Im m\; \partial_e\, \mathbf{E}\, \log\left(\det\left(A_n^e \;+\; B_n^e\,(U_{n-1}^e)^*\right)\right)\;. \tag{47}$$

For a fixed energy, this quantity can also be understood as a rotation number in the sense of Ruelle [Rue]. The second ergodic quantity considered here is the averaged sum of the positive Lyapunov exponents, denoted shortly by $\gamma(E)$ here. For any complex energy $E \in \mathbb{C}$, it can be defined by [CS, BL, KS, CL, SB]

$$\gamma(E) \;=\; \lim_{N\to\infty} \frac{1}{N\,L}\,\mathbf{E}\,\log\left(\left\|\Lambda^L\left(\prod_{n=1}^{N} \mathcal{T}_n^E\right)\right\|\right)\;, \tag{48}$$

where $\Lambda^L\mathcal{T}$ is the L-fold exterior product (second quantization as for evolution group) of the symplectic matrix $\mathcal{T}$, and the norm denotes the operator norm on the fermionic Fock space $\Lambda^L\mathbb{C}^{2L}$. It is well known that $\gamma(E)$ is subharmonic in E [CS, CL]. Furthermore, the Thouless formula linking $\mathcal{N}$ and γ holds [CS, KS]. Actually this is the integrated version of the Kramers-Krönig relation stating that $\gamma(E) + \imath\,\pi\,\mathcal{N}(E)$ for real E is the boundary value of a Herglotz function (which is given by the expectation value of the trace of the logarithm of the Weyl-Titchmarch matrix [KS], for which one has a matrix-valued Herglotz representation [GT]). This is reflected by the following proposition showing that γ and $\pi\,\mathcal{N}$ can be calculated as real and imaginary part of the Birkhoff sum associated to a single complex valued additive cocycle.

Proposition 9 *For E with $\Im m(E) \geq 0$,*

$$\gamma(E) \;=\; \lim_{N\to\infty} \frac{1}{N\,L} \sum_{n=1}^{N} \Re e\;\mathbf{E}\;\log\left(\det\left(A_n^E \;+\; B_n^E\,(U_{n-1}^E)^*\right)\right)\;.$$

Proof. Clearly one may replace $\mathcal{T}_n^E$ in (48) by $\mathcal{M}\mathcal{T}_n^E\mathcal{M}^{-1}$ because the boundary contributions drop out in the limit. Furthermore, instead of calculating the operator norm in (48), one may insert a real Lagrangian plane $\Phi_0 = (\phi_1, \ldots, \phi_L)$ as initial conditions

$$\gamma(E) \;=\; \lim_{N\to\infty} \frac{1}{N\,L}\,\mathbf{E}\;\log\left(\left\|\Lambda^L\left(\prod_{n=1}^{N} \mathcal{M}\,\mathcal{T}_n^E\,\mathcal{M}^{-1}\right)\;\phi_1\wedge\ldots\wedge\phi_L\right\|\right)\;,$$

where now the norm is that of a vector in $\Lambda^L\mathbb{C}^{2L}$ [BL, A.III.3.4] (for covariant, but not necessarily random Jacobi matrices with matrix entries, this holds as long as $\mathbf{E}$ contains an average over Φ_0 w.r.t. some continuous measure [JSS, SB]). Recalling that the norm in $\Lambda^L\mathbb{C}^{2L}$ is calculated with the determinant, it follows that

$$\gamma(E) \;=\; \lim_{N\to\infty}\,\frac{1}{2\,N\,L}\;\mathbf{E}\,\log\left(\det\left(\Phi_0^*\Bigl(\prod_{n=1}^{N}\mathcal{M}\,\mathcal{T}_n^E\,\mathcal{M}^{-1}\Bigr)^*\,\Bigl(\prod_{n=1}^{N}\mathcal{M}\,\mathcal{T}_n^E\,\mathcal{M}^{-1}\Bigr)\Phi_0\right)\right)\,.$$

Now $\left(\prod_{n=1}^N \mathcal{M}\,\mathcal{T}_n^E\,\mathcal{M}^{-1}\right)\Phi_0 = \Phi_N^E$ and one may telescope (boundary terms vanish in the limit) and insert the Cayley transformation:

$$\gamma(E) \;=\; \lim_{N\to\infty}\,\frac{1}{2\,N\,L}\;\mathbf{E}\,\sum_{n=1}^{N}\,\log\left(\frac{\det\bigl((\mathcal{C}\Phi_n^E)^*\,(\mathcal{C}\Phi_n^E)\bigr)}{\det\bigl((\mathcal{C}\Phi_{n-1}^E)^*\,(\mathcal{C}\Phi_{n-1}^E)\bigr)}\right)\,.$$

In each term, one can now apply Lemma 3 for $\mathcal{T} = \mathcal{C}\mathcal{M}\mathcal{T}_n^E\mathcal{M}^{-1}\mathcal{C}^*$ and $\Phi = \mathcal{C}\Phi_{n-1}^E$. The hypothesis of the lemma are indeed satisfied for any E with $\Im m(E)\geq 0$ because of the arguments in Section 2.5. According to the definition of U_n^E, it therefore follows

$$\gamma(E) \;=\; \lim_{N\to\infty}\,\frac{1}{2\,N\,L}\;\mathbf{E}\,\sum_{n=1}^{N}\,\log\left(\frac{\det\bigl((U_n^E)^*\,U_n^E+\mathbf{1}\bigr)}{\det\bigl((U_{n-1}^E)^*\,U_{n-1}^E+\mathbf{1}\bigr)}\;\;\bigl|\det\bigl(A_n^E\,+\,B_n^E\,(U_{n-1}^E)^*\bigr)\bigr|^2\right)\,.$$

The first contribution telescopes back again and the boundary term at N is bounded because $1\leq\det(U^*U+\mathbf{1})\leq 2^L$ for every $U\in\mathbb{D}_L^{\mathbb{C}}\cup\partial_L\mathbb{D}_L^{\mathbb{C}}$. Hence the first contribution vanishes in the limit. The second contribution is precisely the term appearing in the proposition. $\Box$

4.2 Random perturbations

This section gives the precise hypothesis of Theorem 2 and then provides the proof. Hence V_n and T_n are random and depend on a coupling parameter $\lambda\geq 0$ as described in the introduction and they give rise to transfer matrices $\mathcal{T}_n^E(\lambda)$ which depend analytically on λ (lower regularity is actually sufficient). Throughout this section $E\in\mathbb{R}$. The first step of the analysis consists in the symplectic diagonalization of $\mathcal{T}^E=\mathcal{T}_n^E(0)$ by an adequate symplectic basis change $\mathcal{M}$:

$$\mathcal{M}\,\mathcal{T}_n^E(\lambda)\,\mathcal{M}^{-1} \;=\; \mathcal{R}\,\exp\bigl(\lambda\,\mathcal{P}_n\,+\,\mathcal{O}(\lambda^2)\bigr)\,. \tag{49}$$

Here (and in matrix equations below) the expression $\mathcal{O}(\lambda^2)$ means that we have an operator norm estimate on the remainder. Furthermore $\mathcal{P}_n$ is a (random) element of the Lie algebra $\mathrm{sp}(2L,\mathbb{R})$ calculated from (v_n,t_n) and $\mathcal{R}$ is of the symplectic normal form of the free transfer matrix $\mathcal{T}^E$

chosen as follows. The eigenvalues of $\mathcal{T}^E$ form quadruples $(\lambda, 1/\lambda, \overline{\lambda}, 1/\overline{\lambda})$ which collapse to pairs $(\lambda, 1/\lambda)$ if $\lambda \in S^1$ and $\lambda \in \mathbb{R}$. If $\lambda \in S^1$, one speaks of an elliptic channel. Let there be L_e of them, denote their eigenvalues by $e^{\imath\eta_1}, \ldots, e^{\imath\eta_{L_e}}$ and set $\eta = \mathrm{diag}(\eta_1, \ldots, \eta_{L_e})$. As $\mathcal{T}^E$ is supposed to be diagonalizable, the remaining $L_h = L - L_e$ channels are hyperbolic. The moduli of their eigenvalues are $e^{\kappa_l}, e^{-\kappa_l}$, with $\kappa_l > 0$ and for $l = 1, \ldots, L_h$. Set $\kappa = \mathrm{diag}(\kappa_1, \ldots, \kappa_{L_h})$. If a hyperbolic channel stems from a quadruple, it moreover contains a rotation by the phase of its eigenvalue λ. This will be described by $S \in \mathrm{O}(L_h)$ which is a tridiagonal orthogonal matrix containing only either 1 or 2×2 rotation matrices on the diagonal and which satisfies $[S, e^\kappa] = 0$. The symplectic basis change $\mathcal{M}$ is then chosen such that

$$\mathcal{R} \;=\; \begin{pmatrix} S\,e^{\kappa} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \cos(\eta) & \mathbf{0} & \sin(\eta) \\ \mathbf{0} & \mathbf{0} & S\,e^{-\kappa} & \mathbf{0} \\ \mathbf{0} & -\sin(\eta) & \mathbf{0} & \cos(\eta) \end{pmatrix} \,,$$

Furthermore, let P_h and P_e denote the projections ($L \times L$ matrices) onto the hyperbolic and elliptic channels. In particular, $P_h + P_e = \mathbf{1}$ and $\mathrm{diag}(P_h, P_h)$ as well as $\mathrm{diag}(P_e, P_e)$ commute with $\mathcal{R}$. The reader may consult [SB] where the basis change $\mathcal{M}$ is constructed explicitly for the example of the Anderson model on a strip. Next let us state the precise hypothesis of Theorem 2.

Hypothesis: *The expansion factors κ_l and rotation phases η_l satisfy*

$$g_h \;=\; \min_{1\leq l\leq L_h} \,(1 - e^{-\kappa_l}) \;>\; 0\;, \qquad g_e \;=\; \min_{1\leq l,k\leq L_e} \left|1 - e^{\imath(\eta_l+\eta_k)}\right| \;>\; 0\;.$$

In order to develop the perturbation theory, some further notations are needed:

$$\mathcal{C}\,\mathcal{M}\,\mathcal{T}_n^E(\lambda)\,\mathcal{M}^{-1}\,\mathcal{C}^* \;=\; \begin{pmatrix} A_n^E(\lambda) & B_n^E(\lambda) \\ \overline{B_n^E(\lambda)} & \overline{A_n^E(\lambda)} \end{pmatrix} \;=\; \begin{pmatrix} A + \lambda a_n & B + \lambda b_n \\ \overline{B + \lambda b_n} & \overline{A + \lambda a_n} \end{pmatrix} \;+\; \mathcal{O}(\lambda^2)\;.$$

Comparing with (49), one checks that

$$A \;=\; \begin{pmatrix} S\,\cosh(\kappa) & \mathbf{0} \\ \mathbf{0} & e^{\imath\eta} \end{pmatrix}\,, \qquad B \;=\; \begin{pmatrix} S\,\sinh(\kappa) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}\,, \qquad A \pm B \;=\; \begin{pmatrix} e^{\pm\kappa} & \mathbf{0} \\ \mathbf{0} & e^{\imath\eta} \end{pmatrix}\,,$$

and

$$a_n \;=\; \begin{pmatrix} A \\ B \end{pmatrix}^t \mathcal{C}\,\mathcal{P}_n\,\mathcal{C}^* \begin{pmatrix} \mathbf{1} \\ \mathbf{0} \end{pmatrix}\,, \qquad b_n \;=\; \begin{pmatrix} A \\ B \end{pmatrix}^t \mathcal{C}\,\mathcal{P}_n\,\mathcal{C}^* \begin{pmatrix} \mathbf{0} \\ \mathbf{1} \end{pmatrix}\,.$$

Note that both A and B commute with both P_h and P_e.

According to Section 4.1, the averaged Lyapunov exponent and IDS at a real energy E for the λ-dependent random operators $H^N(\lambda)$ are given by

$$\gamma_\lambda(E) \;+\; \imath\,\pi\,\mathcal{N}_\lambda(E) \;=\; \lim_{N\to\infty} \frac{1}{N\,L} \sum_{n=1}^{N} \int_{-\infty}^{E} de\; \partial_e\, \mathbf{E}\; \log\big(\det\big(\,A_n^e(\lambda) \;+\; B_n^e(\lambda)\,(U_{n-1}^e(\lambda))^*\,\big)\big)\;.$$

Let us expand the integrand

$$\log\big(\det\big(\,A_n^E(\lambda) \;+\; B_n^E(\lambda)\,(U_{n-1}^E(\lambda))^*\,\big)\big) \;=\; \log\big(\det\big(\,A_n^E(\lambda) \;+\; B_n^E(\lambda)\,P_h\,\big)\big) \;+\; J_n(\lambda)\;, \qquad (50)$$

where

$$J_n(\lambda) \;=\; \mathrm{Tr}\,\big(\log\big(\,\mathbf{1} \;+\; (A_n^E(\lambda) \;+\; B_n^E(\lambda)\,P_h)^{-1} B_n^E(\lambda)\,(U_{n-1}^E(\lambda) - P_h)^*\,\big)\big)\;, \qquad (51)$$

which is possible because $A_n^E(\lambda) + B_n^E(\lambda)\,P_h = A + B + \mathcal{O}(\lambda)$ is invertible for λ sufficiently small. Note that only $J_n(\lambda)$ depends on U_{n-1}^E, while the first contribution gives an contribution to IDS and Lyapunov exponent which can be readily calculated, similar as in (44). Hence we need to focus on the control of Birkhoff averages of $J_n(\lambda)$. For this purpose, one would first like to expand the logarithm in (51). As $B_n^E(\lambda) = BP_h + \mathcal{O}(\lambda)$, one therefore has to show that $P_h U_n^E(\lambda) - P_h$ is small in norm. This means that the hyperbolic part of the dynamics (at $\lambda = 0$) alines $P_h U_n^E(\lambda)$ deterministically with P_h up to small corrections due to the random perturbation. The following lemma is a strengthening of prior results [SB] on this dynamical separation of hyperbolic and elliptic channels.

Lemma 7 *Let $U_0^E = \mathbf{1}$ (choice of initial condition). Then there exist positive constants c_1, c_2 such that for $\lambda < \frac{g_h^2}{4c_1c_2}$ and all $n \geq 1$, one has*

$$\|\, P_h U_n^E(\lambda) - P_h \,\| \;\leq\; \frac{2\,c_1\,\lambda}{g_h}\;.$$

Proof. For sake of notational simplicity, let P denote P_h within this proof. Let U be a symmetric unitary and set $U' = \mathcal{C}\mathcal{M}\mathcal{T}_n^E(\lambda)\mathcal{M}^{-1}\mathcal{C}^* \cdot U$. We will show that uniformly in n holds

$$\|\, PU' - P \,\| \;\leq\; (1 - g_h)\,\|\, PU - P \,\| \;+\; c_1\,\lambda \;+\; c_2\,\|\, PU - P \,\|^2\;. \qquad (52)$$

An elementary dynamical argument then allows to conclude the proof (the constants c_1 and c_2 are then the same as in the statement of the lemma). In order to prove (52), let us first note that $\lambda \mapsto \mathcal{C}\mathcal{M}\mathcal{T}_n^E(\lambda)\mathcal{M}^{-1}\mathcal{C}^* \cdot U$ is an analytic path of unitaries. Hence the eigenvalues vary analytically in λ [Kat]. Therefore $U' = \mathcal{C}\mathcal{R}\mathcal{C}^* \cdot U + R_1$ where R_1 depends on U and $\mathcal{T}_n^E(\lambda)$, but one has the norm bound $\|R_1\| \leq c_1\lambda$ uniformly in n and U (because of the uniform bounds on the norms of $\mathcal{P}_n$ and the error terms in (49)). Therefore it is sufficient to show (52) for $\lambda = 0$.

By definition of the Möbius action, $U' = (AU + B)(BU + \overline{A})^{-1}$ so that

$$PU' \;=\; P\big(A(PU-P) \,+\, (A+B)\big)\,(\overline{A}+B)^{-1}\,\big(\mathbf{1} \,+\, B\,(PU-P)\,(\overline{A}+B)^{-1}\big)^{-1} .$$

Now one can expand the last inverse in $(PU - P)$ to first order, with an error term bounded by $\|PU - P\|^2$. Then multiplying out all the remaining factors shows that

$$PU' - P \;=\; P\,(A-B)\,(PU-P)\,(\overline{A}+B)^{-1} \;+\; R_2\,, \tag{53}$$

with an error term that satisfies $\|R_2\| \leq c_2\,\|PU-P\|^2$. Now $\|(\overline{A}+B)^{-1}\| = 1$ and $\|P(A-B)\| = \max_{1\leq l\leq L_h}\, e^{-\kappa_l} = 1 - g_h$ which implies (52) for $\lambda = 0$. $\square$

Now it is possible to expand the logarithm in (51) because $B^E_n(\lambda)P_e = \mathcal{O}(\lambda)$ so that Lemma 7 implies $B^E_n(\lambda)(U^E_{n-1}(\lambda) - P_h)^* = \mathcal{O}(\lambda)$ (here still all error terms are norm bounded). Hence

$$J_n(\lambda) \;=\; \mathrm{Tr}\,\Big(\,(A^E_n(\lambda) \,+\, B^E_n(\lambda)\,P_h)^{-1}B^E_n(\lambda)\,(U^E_{n-1}(\lambda) - P_h)^*\,\Big) \;+\; \mathcal{O}\Big(\frac{L\lambda^2}{g_h^2}\Big)\,,$$

where the L comes from carrying out the trace after having applied the norm bound. Expanding $A^E_n(\lambda)$ and $B^E_n(\lambda)$, using the commutativity of A and B with P_h and P_e and invoking Lemma 7 in order to show $P_hU^E_n(\lambda)P_e = \mathcal{O}(\lambda/g_h)$ now implies

$$J_n(\lambda) \;=\; \mathrm{Tr}\Big(\,(A+B)^{-1}\big((P_hU^E_{n-1}(\lambda)^*P_h - P_h) \;+\; \lambda\, b_n\, P_eU^E_{n-1}(\lambda)^*P_e\big)\Big) \;+\; \mathcal{O}\Big(\frac{L\lambda^2}{g_h^2}\Big) .$$

Setting

$$I_h(N) \;=\; \mathbf{E}\,\frac{1}{N\,L}\,\sum_{n=0}^{N-1}\,(P_hU^E_n(\lambda)P_h \;-\; P_h)\,, \qquad I_e(N) \;=\; \mathbf{E}\,\frac{1}{N\,L}\,\sum_{n=0}^{N-1}\,P_e\,U^E_n(\lambda)P_e\,,$$

one has

$$\mathbf{E}\,\frac{1}{N\,L}\,\sum_{n=1}^{N}\,J_n(\lambda) \;=\; \mathrm{Tr}\,\big(\,(A+B)^{-1}I_h(N)^*\,\big) \;+\; \lambda\,\mathrm{Tr}\,\big(\,(A+B)^{-1}\mathbf{E}_\sigma(b_\sigma)\,I_e(N)^*\,\big) \;+\; \mathcal{O}\Big(\frac{\lambda^2}{g_h^2}\Big) .$$

In order to calculate and bound the two traces, we will use the Hilbert-Schmidt spaces $\mathcal{H}_h$ and $\mathcal{H}_e$ of complex matrices respectively of size $L_h \times L_h$ and $L_e \times L_e$, furnished with the scalar product $\langle C|D\rangle_2 = \mathrm{Tr}(C^*D)$. The corresponding norms are $\|C\|_2 = \mathrm{Tr}(C^*C)^{\frac{1}{2}}$. They satisfy norm the inequality $\|C\|_2 \le \sqrt{L}\ \|C\|$ w.r.t. to the operator norm (where one may, of course, also use respectively L_h and L_e instead of L). For a $L \times L$ matrix C, we will identify $P_h C P_h$ and $P_e C P_e$ with vectors in respectively $\mathcal{H}_h$ and $\mathcal{H}_e$. Let us first focus on the second trace in the last expression. The Cauchy-Schwarz inequality implies

$$\mathrm{Tr}\left((A+B)^{-1}\,\mathbf{E}_\sigma(b_\sigma)\,I_e(N)^*\right) \;\le\; \sqrt{L}\,\|P_e(A+B)^{-1}\,\mathbf{E}_\sigma(b_\sigma)P_e\|\;\|I_e(N)\|_2\,.$$

As the operator norm appearing on the r.h.s. is bounded, the following lemma shows that this trace is of order $\mathcal{O}(\lambda/\sqrt{L})$ and hence does not contribute to leading order.

Lemma 8 *There exist positive constants c_1 and c_2 such that*

$$\|I_e(N)\|_2 \;\le\; \frac{1}{g_e\sqrt{L}}\,\left(c_1\,\lambda \;+\; c_2\,\frac{1}{N}\right)\,.$$

Proof. This is a matrix version of the oscillatory sum argument in [PF, SB]. First note that for each summand in $I_e(N)$, one has $P_e\,U_n^E(\lambda)P_e = e^{\imath\eta}P_e\,U_{n-1}^E(\lambda)P_e e^{\imath\eta} + \mathcal{O}(\lambda)$. Thus

$$I_e(N) \;=\; e^{\imath\eta}\,I_e(N)\,e^{\imath\eta} \;+\; R_1 \;+\; R_2\,,$$

with an average error term R_1 satisfying $\|R_1\| \le c_1\,\lambda/L$ and boundary terms R_2 satisfying $\|R_2\| \le c_2/(NL)$. Now let us define the super-operator $D_\eta : \mathcal{H}_e \to \mathcal{H}_e$ by $D_\eta(C) = e^{\imath\eta}Ce^{\imath\eta}$. This operator is diagonal and the hypothesis $g_e > 0$ implies that $(\mathbf{1} - D_\eta)^{-1}$ exists and its norm is bounded by $1/g_e$. As $I_e(N) = (\mathbf{1}-D_\eta)^{-1}(R_1+R_2)$, it follows that $\|I_e(N)\|_2 \le (\|R_1\|_2+\|R_2\|_2)/g_e$ which leads to the desired bound. □

A similar argument allows to calculate the remaining trace.

Lemma 9 *One has*

$$\mathrm{Tr}\left((A+B)^{-1}I_h(N)^*\right) \;=\; 2\,\lambda\,\Re e\;\mathrm{Tr}\left((e^{2\kappa} - \mathbf{1})^{-1}P_h\,\mathbf{E}_\sigma(a_\sigma + b_\sigma)\,P_h\right) \;+\; \mathcal{O}\left(\frac{\lambda^2}{g_h^3}\,,\,\frac{1}{g_h\,N}\right)\,.$$

Proof. One first has to refine (53) and include the $\mathcal{O}(\lambda)$ contribution. Invoking Lemma 7 at several reprises, some lengthy but straightforward algebra shows

$$P_h U_n^E(\lambda)P_h - P_h \;=\; S\,e^{-\kappa}\,(P_h U_{n-1}^E(\lambda)P_h - P_h)\,e^{-\kappa}\,S^t \;+\; 2\,\lambda\,\Re e\;P_h\,\mathbf{E}_\sigma(a_\sigma + b_\sigma)\,P_h\,e^{-\kappa}\,S^t \;+\; L\,R_1\,,$$

with $\|R_1\| \le c_1\,\lambda^2/(Lg_h^2)$ and the formula is understood as identity for operators on $\mathcal{H}_h$. Now define the super-operator $D_\kappa : \mathcal{H}_h \to \mathcal{H}_h$ by $D_\kappa(C) = Se^{-\kappa}Ce^{-\kappa}S^t$. One directly checks $\|(\mathbf{1} - D_\kappa)^{-1}\| \le 1/g_h$. As above,

$$I_h(N) \;=\; (\mathbf{1} - D_\kappa)^{-1}\Big(\frac{2\,\lambda}{L}\;\Re e\;P_h\,\mathbf{E}_\sigma(a_\sigma + b_\sigma)\,P_h\,e^{-\kappa}\,S^t \;+\; R_1 \;+\; R_2\Big)\,,$$

where $\|R_2\| \leq c_2/(NL)$. Replacing this into the trace and bounding the error terms by the Cauchy-Schwarz inequality just as before Lemma 8 allows to bound the error terms. The leading order contribution can be calculated using the identity

$$S^t\, e^{-\kappa}\, (\mathbf{1} - D_\kappa^*)^{-1}(S\, e^{-\kappa}) \;=\; (e^{2\kappa} - 1)^{-1}\;.$$

This completes the proof. $\square$

Replacing Lemma 9, it then follows that

$$\begin{aligned}\gamma_\lambda(E) \;+\; \imath\,\pi\,\mathcal{N}_\lambda(E) \;\;&=\;\; \mathbf{E}_\sigma\,\frac{1}{L}\int_{-\infty}^{E} de\;\partial_e\;\log\big(\det\big(\,A^e_\sigma(\lambda)\;+\;B^e_\sigma(\lambda)\,P_h\,\big)\,\big)\\ &\quad+\frac{2\,\lambda}{L}\,\Re e\;\mathrm{Tr}\,\big(\,(e^{2\kappa}-\mathbf{1})^{-1}P_h\,\mathbf{E}_\sigma(a_\sigma+b_\sigma)\;P_h\,\big)\;+\;\mathcal{O}\left(\frac{\lambda^2}{g_e}\,,\,\frac{\lambda^2}{g_h^3}\right)\;.\end{aligned} \tag{54}$$

As this holds also for the translation invariant operator with one fixed σ at every site n (which has non-random independent entries), one deduces

$$\gamma_\lambda(E) \;+\; \imath\,\pi\,\mathcal{N}_\lambda(E) \;=\; \mathbf{E}_\sigma\;\gamma_{\lambda,\sigma}(E) \;+\; \imath\,\pi\;\mathbf{E}_\sigma\;\mathcal{N}_{\lambda,\sigma}(E) \;+\; \mathcal{O}\left(\frac{\lambda^2}{g_e}\,,\,\frac{\lambda^2}{g_h^3}\right)\;,$$

where $\gamma_{\lambda,\sigma}(E)$ and $\mathcal{N}_{\lambda,\sigma}(E)$ are averaged Lyapunov exponent and IDS of the translation invariant operator (as already described in the introduction). This therefore proves Theorem 2. Expanding the logarithm in (54), some straightforward algebra leads to more explicit perturbative formulas for $\gamma_\lambda(E)$ and $\mathcal{N}_\lambda(E)$ in terms of $\mathbf{E}_\sigma(\mathcal{P}_\sigma)$. Let us note that the contribution of Lemma 9 is real and hence only contributes to $\gamma_\lambda(E)$. The lowest order contribution to $\mathcal{N}_\lambda(E)$ is given by the first term in (50) and one can check that it is only the contribution of $\mathbf{E}(\mathcal{P}_\sigma)$ which changes the rotation phases of the elliptic channels of $\mathcal{R}$.

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