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An atlas for tridiagonal isospectral manifolds

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Abstract

Let $\mathscr{T}_\Lambda$ be the compact manifold of real symmetric tridiagonal matrices conjugate to a given diagonal matrix Λ with simple spectrum. We introduce *bidiagonal coordinates*, charts defined on open dense domains forming an explicit atlas for $\mathscr{T}_\Lambda$. In contrast to the standard inverse variables, consisting of eigenvalues and norming constants, every matrix in $\mathscr{T}_\Lambda$ now lies in the interior of some chart domain. We provide examples of the convenience of these new coordinates for the study of asymptotics of isospectral dynamics, both for continuous and discrete time.

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1. Introduction

Let Λ be a real diagonal matrix with simple spectrum and $\mathscr{T}_\Lambda$ be the manifold of real, symmetric, tridiagonal matrices having the same spectrum as Λ. The purpose of this paper is to present an explicit atlas for $\mathscr{T}_\Lambda$: the charts in the atlas define the *bidiagonal coordinates* on open dense subsets of $\mathscr{T}_\Lambda$. As is familiar to numerical analysts, many algorithms to compute spectra operate by iteration on Jacobi matrices, yielding approximations of reduced tridiagonal matrices. Given

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a limit point p for such iterations, there is a chart in the atlas containing p in its interior, reducing the study of asymptotic behavior to a matter of local theory. The construction of the atlas was motivated by our study of the asymptotics of the Wilkinson shift iteration: we use bidiagonal coordinates to prove that this well known algorithm deflates cubically for generic spectra [10] but only quadratically for certain initial conditions [11].

Jacobi matrices are frequently parameterized by its (simple) eigenvalues and the vector w of (positive) first coordinates of its normalized eigenvectors, the *norming constants*. An algorithm to recover a Jacobi matrix from these data was known to Stieltjes [13]. From the procedure, one learns that the set $\mathscr{J}_\Lambda \subset \mathscr{T}_\Lambda$ of Jacobi matrices with prescribed simple spectrum is diffeomorphic to $\mathbb{R}^{n-1}$. Norming constants break down at the boundary of $\mathscr{J}_\Lambda$, and new techniques are required to study its closure $\overline{\mathscr{J}_\Lambda}$ within the space of symmetric matrices. In [19], $\overline{\mathscr{J}_\Lambda}$ was proved to be homeomorphic to a convex polytope $\mathscr{P}_\Lambda$ and the boundary of $\overline{\mathscr{J}_\Lambda}$ was described as a union of cells of reduced tridiagonal matrices. But one may go beyond: by making all possible changes of sign along the off-diagonal entries $(i+1, i)$ of the matrices in $\overline{\mathscr{J}_\Lambda}$, one obtains 2^{n-1} copies of $\overline{\mathscr{J}_\Lambda}$, which glue along their boundaries to form the compact manifold $\mathscr{T}_\Lambda$.

There are significant theoretical advantages for considering the manifold $\mathscr{T}_\Lambda$ instead of $\mathscr{J}_\Lambda$ or even $\overline{\mathscr{J}_\Lambda}$. In algorithms to compute the spectrum of Jacobi matrices, the limit point is usually a reduced matrix: if the limit point lies in the interior of the domain, asymptotic behavior becomes amenable to local theory. Furthermore, signs of off-diagonal entries are often dropped in such algorithms. This procedure, which is computationally practical, may introduce theoretical complications akin to inserting absolute values on a smooth function. Enlarging the domain of such iterations to $\mathscr{T}_\Lambda$ may allow for a choice of signs which respects smoothness: one is then entitled to use Taylor expansions in the local study of the iteration.

The bidiagonal coordinates β_i^π, $i = 1, \ldots, n-1$, which play the role of generalized norming constants, are defined on a cover $\mathscr{U}_\Lambda^\pi$ of open dense subsets of $\mathscr{T}_\Lambda$ indexed by permutations $\pi \in S_n$. On each $\mathscr{U}_\Lambda^\pi$, the bidiagonal coordinates give rise to a chart of the atlas, i.e., a diffeomorphism to $\psi_\pi : \mathscr{U}_\Lambda^\pi \to \mathbb{R}^{n-1}$. The underlying construction is easy to describe. A matrix M is *LU-positive* if it admits a (unique) factorization $M = LU$ where L is lower unipotent (i.e., lower triangular with unit diagonal) and U is upper triangular with positive diagonal entries. Set $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n), \lambda_1 < \cdots < \lambda_n$ and, for $\pi \in S_n$, let $\Lambda^\pi = \operatorname{diag}(\lambda_{\pi(1)}, \ldots, \lambda_{\pi(n)})$. A matrix $T \in \mathscr{T}_\Lambda$ belongs to $\mathscr{U}_\Lambda^\pi$ if it admits a diagonalization $T = Q_\pi^* \Lambda^\pi Q_\pi$ for some orthogonal LU-positive matrix $Q_\pi = L_\pi U_\pi$; in particular, $\Lambda^\pi \in \mathscr{U}_\Lambda^\pi$. Now set $B_\pi = L_\pi^{-1} \Lambda^\pi L_\pi = U_\pi T U_\pi^{-1}$. From the formulae, B_π is simultaneously lower triangular and upper Hessenberg, hence lower bidiagonal. The construction of the chart is complete:

$$B_\pi = \begin{pmatrix} \lambda_{\pi(1)} & & & & \\ \beta_1^\pi & \lambda_{\pi(2)} & & & \\ & \beta_2^\pi & \lambda_{\pi(3)} & & \\ & & \ddots & \ddots & \\ & & & \beta_{n-1}^\pi & \lambda_{\pi(n)} \end{pmatrix}, \quad \psi_\pi(T) = \left(\beta_1^\pi, \ldots, \beta_{n-1}^\pi\right).$$

It turns out that if $T \in \mathscr{T}_\Lambda$ is unreduced then $T \in \mathscr{U}_\Lambda^\pi$ for all $\pi \in S_n$ (Lemma 3.2).

As far as we know, this construction of the matrices L_π and B_π was first used by Terwilliger in his study of Leonard pairs [17]; our matrix L_π, for example, appears in his Lemma 4.4 as E_r. Carnicer and Peña [3] also consider changes of basis leading to bidiagonal matrices in their study of oscillatory matrices.

For Jacobi matrices, bidiagonal coordinates are, up to a multiplicative factor, quotients of norming constants (Proposition 3.6):

$$\beta_i^\pi = \left| \frac{(\lambda_{\pi(i+1)} - \lambda_{\pi(1)}) \cdots (\lambda_{\pi(i+1)} - \lambda_{\pi(i)})}{(\lambda_{\pi(i)} - \lambda_{\pi(1)}) \cdots (\lambda_{\pi(i)} - \lambda_{\pi(i-1)})} \right| \frac{w_{\pi(i+1)}}{w_{\pi(i)}}, \quad 1 \leqslant i \leqslant n-1,$$

where $w_{\pi(i)} = |(Q_\pi)_{i,1}|$. Norming constants, however, yield no chart for a neighborhood of a diagonal matrix in $\mathscr{T}_\Lambda$. Bidiagonal coordinates imply that in $\mathscr{U}_\Lambda^\pi$ appropriate quotients of norming constants $w_{\pi(i+1)}/w_{\pi(i)}$ admit natural smooth extensions, a fact discussed in [7] and [12]. There is however no satisfactory definition for the sign of norming constants for matrices throughout $\mathscr{T}_\Lambda$: this will be discussed more carefully at the end of Section 2.

In the next two sections, we consider the theoretical setup. Section 2 contains some basic facts about Jacobi matrices and norming constants, presented using the concept of LU-positivity so as to prepare the reader to the discussion of bidiagonal coordinates. We also collect some geometric properties of the isospectral manifold $\mathscr{T}_\Lambda$: the case $n = 3$ is taken as a detailed example. In Section 3, we describe the domains $\mathscr{U}_\Lambda^\pi$ both in terms of LU-positivity and based on a cell decomposition of $\mathscr{T}_\Lambda$. We then construct the charts $\psi_\pi : \mathscr{U}_\Lambda^\pi \to \mathbb{R}^{n-1}$ and their inverses ϕ_π: the bidiagonal coordinates for $T \in \mathscr{U}_\Lambda^\pi$ are $(\beta_1^\pi, \ldots, \beta_{n-1}^\pi) = \psi_\pi(T)$. We also prove that the quotients $\beta_i^\pi/((T)_{i+1,i})$ are smooth strictly positive functions in $\mathscr{U}_\Lambda^\pi$.

In order to provide applications, we concentrate on two kinds of dynamics acting on Jacobi matrices: *QR steps* (Section 4) and *Toda flows* (Section 5). Algorithms to compute eigenvalues of Jacobi matrices which are related to the QR factorization, as well as the flows in the *Toda hierarchy*, admit a very simple description in bidiagonal coordinates: they evolve linearly in time. From this description, limits at infinity (with asymptotic rates) are immediate. As a slightly more complicated example, we prove the cubic convergence of the Rayleigh quotient shift iteration using a Taylor expansion. More precisely, given Λ, let $G(T) \in \mathscr{T}_\Lambda$ be obtained from $T \in \mathscr{T}_\Lambda$ by a Rayleigh quotient step: we prove that there exist $c, \epsilon > 0$ such that if $|(T)_{n,n-1}| < \epsilon$ then $|(G(T))_{n,n-1}| < \min(\epsilon, c|(T)_{n,n-1}|^3)$. The reader should compare this argument with the more complicated study of the asymptotics of the Wilkinson's shift iteration in [10,11]. We conclude the paper with the computation of the *wave and scattering maps* of the standard Toda flow, a physical system consisting of n particles on the line under the influence of a special Hamiltonian. Moser [13] had previously computed the scattering map and Percy Deift (personal communication) the wave map, but our arguments are significantly different.

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2. Tridiagonal matrices

We begin this section by sketching some classical facts about tridiagonal matrices [13,14] in a phrasing appropriate to our purposes. Let $\mathscr{T}$ be the vector space of real, tridiagonal, $n \times n$ symmetric matrices. A matrix $T \in \mathscr{T}$ is *Jacobi* (resp. *unreduced*) if $T_{i+1,i} > 0$ (resp. $T_{i+1,i} \neq 0$) for $i = 1, 2, \ldots, n-1$. Let $\mathscr{J} \subset \mathscr{T}$ be the open cone of Jacobi matrices and $\mathbb{R}_o^n$ be the open cone $\{(x_1, \ldots, x_n), x_1 < \cdots < x_n\}$. The *ordered spectrum map* σ_o is defined on the open set of real symmetric matrices with simple spectrum: $\sigma_o(S) = (\lambda_1, \ldots, \lambda_n) \in \mathbb{R}_o^n$ lists the eigenvalues of S in increasing order. Let $O(n)$ be the group of real orthogonal matrices of order n. For an invertible M, write the unique *QR factorization* $M = \mathbf{Q}(M)\mathbf{R}(M)$, for $\mathbf{Q}(M) \in O(n)$ and $\mathbf{R}(M)$ upper triangular with positive diagonal. Similarly, when the leading principal minors of M are invertible, write the *LU factorization* $M = \mathbf{L}(M)\mathbf{U}(M)$ where $\mathbf{L}(M)$ is lower unipotent (i.e., lower triangular with unit diagonal) and $\mathbf{U}(M)$ is upper triangular.

For a permutation $\pi \in S_n$, consider the matrix P_π with (i, j) entry equal 1 if and only if $i = \pi(j)$ (thus $P_{\pi_1\pi_2} = P_{\pi_1}P_{\pi_2}$ and $P_\pi e_i = e_{\pi(i)}$). For $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$, with $\lambda_1 < \cdots < \lambda_n$, set

$$\Lambda^\pi = P_\pi^{-1}\Lambda P_\pi = \operatorname{diag}(\lambda_{\pi(1)}, \lambda_{\pi(2)}, \ldots, \lambda_{\pi(n)}) = \operatorname{diag}(\lambda_1^\pi, \lambda_2^\pi, \ldots, \lambda_n^\pi).$$

Finally, let $\mathscr{E} \subset O(n)$ be the group of *sign diagonals*, i.e., matrices of the form $E = \operatorname{diag}(\pm 1, \pm 1, \ldots, \pm 1)$.

Definition 2.1. A square matrix M is *LU-positive* if $\mathbf{U}(M)$ is well defined and the diagonal entries of $\mathbf{U}(M)$ are positive. Given $T \in \mathscr{T}$, $\Lambda = \operatorname{diag}(\sigma_o(T))$ and a permutation π, the factorization $T = Q_\pi^* \Lambda^\pi Q_\pi$ is a *π-normalized diagonalization* if the orthogonal matrix Q_π is LU-positive.

Equivalently, M is LU-positive if the determinants of its leading principal minors are positive. The π-normalized diagonalization of $T \in \mathscr{T}$ is unique if it exists. Indeed, two factorizations $Q_1^*\Lambda^\pi Q_1 = Q_2^*\Lambda^\pi Q_2$ yield $Q_2 = EQ_1$ for some $E \in \mathscr{E}$, Q_1 and Q_2 both LU-positive: we must have $E = I$.

We recast a standard result for our purposes.

Theorem 2.2. *The eigenvalues of a Jacobi matrix J are distinct. Given J and a permutation $\pi \in S_n$, J admits a (unique) π-normalized diagonalization $J = Q_\pi^*\Lambda^\pi Q_\pi$ where $\Lambda = \operatorname{diag}(\sigma_o(J))$. The coordinates of $Q_\pi e_1$ are nonzero. The map below is a diffeomorphism*:

$$\begin{aligned}\Gamma_\pi : \mathscr{J} &\to \mathbb{R}^n_o \times \{w \in \mathbb{R}^n \,|\, \|w\| = 1, w_i > 0\}\\ J &\mapsto (\sigma_o(J), (|(Q_\pi)_{11}|, |(Q_\pi)_{21}|, \ldots, |(Q_\pi)_{n1}|)).\end{aligned}$$

The second entry w of $\Gamma_\pi(J)$ lists the *norming constants* of J. For different $\pi \in S_n$, the coordinates of w are merely permuted. Indeed, if $J = Q^*\Lambda Q$ and $J = Q_\pi^*\Lambda^\pi Q_\pi$ then $Q_\pi = EP_\pi^{-1}Q$ for some $E \in \mathscr{E}$.

Proof. Simplicity of the spectrum of J and the fact that the first coordinate of each eigenvector is nonzero are standard facts [14]. In other words, given a diagonalization $J = \widetilde{Q}^*\Lambda^\pi\widetilde{Q}$, the coordinates of $\tilde{w} = \widetilde{Q}e_1$ are nonzero. Clearly, the matrices $\widehat{Q} \in \mathrm{O}(n)$ for which $J = \widehat{Q}^*\Lambda^\pi\widehat{Q}$ are of the form $\widehat{Q} = E\widetilde{Q}$ for a sign diagonal $E \in \mathscr{E}$, i.e., we may change signs of rows of $\widetilde{Q}$. The values of $|(\widehat{Q})_{i1}|$ do not depend on the choice of $\widehat{Q}$ thus allowing us to define the smooth map Γ_π using any diagonalization (not necessarily π-normalized). We show that one such matrix $\widehat{Q}$ is LU-positive and that Γ_π is a diffeomorphism by constructing the inverse of Γ_π.

Construct a Vandermonde matrix V with $V_{ij} = \lambda_{\pi(i)}^{j-1}$ and a positive diagonal matrix $\widetilde{W} = \operatorname{diag}(\tilde{w}_1, \ldots, \tilde{w}_n)$. The well known formula for the determinant of a Vandermonde matrix implies that the leading principal minors of V are nonzero. Thus, there exists a unique sign diagonal $E \in \mathscr{E}$ such that EV is LU-positive: the matrices $E\widetilde{W}V = \widetilde{W}EV$ and $\widetilde{Q} = \mathbf{Q}(E\widetilde{W}V)$ are therefore also LU-positive. We claim that $\widetilde{J} = \widetilde{Q}^*\Lambda^\pi\widetilde{Q}$ is a Jacobi matrix.

To prove tridiagonality, we show that $\widetilde{J}_{ij} = \langle \widetilde{J}e_j, e_i\rangle = \langle \Lambda^\pi\widetilde{Q}e_j, \widetilde{Q}e_i\rangle$ equals 0 for $i > j + 1$. For $j = 1, \ldots, n$, consider the columns $u_j = (\Lambda^\pi)^{j-1}E\tilde{w}$ and $\tilde{q}_j$ of $E\widetilde{W}V$ and $\widetilde{Q}$, respectively. The Krylov subspace K_j spanned by $u_1, \ldots, u_j$ is also spanned by the orthonormal vectors $\tilde{q}_1, \ldots, \tilde{q}_j$ since $\widetilde{Q}\widetilde{R} = E\widetilde{W}V$ where $\widetilde{R} = \mathbf{R}(E\widetilde{W}V)$ is upper triangular with positive diago-

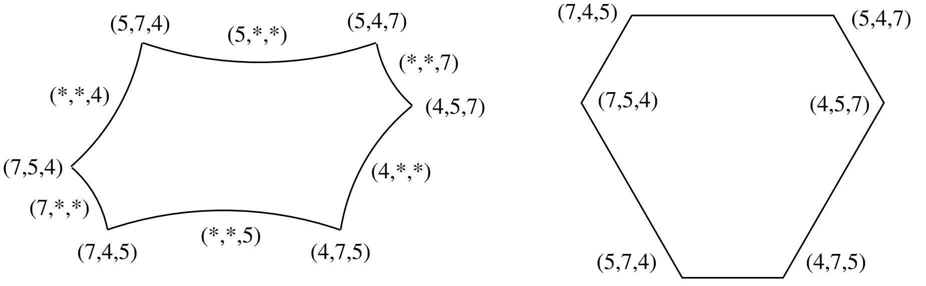

Fig. 1. The spaces $\overline{\mathscr{J}_\Lambda}$ and $\mathscr{P}_\Lambda$ for $\Lambda = \mathrm{diag}(4, 5, 7)$.

nal. We have $\Lambda^\pi K_j \subset K_{j+1}$ and therefore $\Lambda^\pi \tilde{q}_j$ is a linear combination of $\tilde{q}_1, \ldots, \tilde{q}_{j+1}$ and $\langle \Lambda^\pi \tilde{q}_j, \tilde{q}_i \rangle = 0$ as needed.

We now show that $\widetilde{J}_{j+1,j} > 0$. The factorization $\widetilde{Q}\widetilde{R} = E\widetilde{W}V$ implies that $\tilde{q}_i - (\widetilde{R}_{ii})^{-1}u_i \in K_{i-1}$ and similarly $u_{i+1} - \widetilde{R}_{i+1,i+1}\tilde{q}_{i+1} \in K_i$. Applying Λ^π to the first relation we have $\Lambda^\pi \tilde{q}_i - (\widetilde{R}_{ii})^{-1}u_{i+1} \in K_i$ and using the second relation we obtain $\Lambda^\pi \tilde{q}_i - (\widetilde{R}_{ii})^{-1}\widetilde{R}_{i+1,i+1}\tilde{q}_{i+1} \in K_i$. Now, since $K_i \perp \tilde{q}_{i+1}$, we have $\widetilde{J}_{j+1,j} = \langle \Lambda^\pi \tilde{q}_i, \tilde{q}_{i+1} \rangle = (\widetilde{R}_{ii})^{-1}\widetilde{R}_{i+1,i+1}\langle \tilde{q}_{i+1}, \tilde{q}_{i+1} \rangle = (\widetilde{R}_{ii})^{-1}\widetilde{R}_{i+1,i+1} > 0$.

Adding up, $\widetilde{J} = \widetilde{Q}^* \Lambda^\pi \widetilde{Q}$ is the π-normalized diagonalization of the Jacobi matrix $\widetilde{J}$. From this construction, the inverse of Γ_π is smooth, completing the proof. □

Let $\mathscr{J}_\Lambda \subset \mathscr{J}$ be the set of Jacobi matrices J with $\mathrm{diag}(\sigma_o(J)) = \Lambda$: norming constants (or, more precisely, the second coordinate w of Γ_π) obtain a diffeomorphism between $\mathscr{J}_\Lambda$ and the positive orthant of the unit sphere $\{w \in \mathbb{R}^n \| \|w\|\| = 1, w_i > 0\}$. Let $\overline{\mathscr{J}_\Lambda}$ be the closure of $\mathscr{J}_\Lambda$ in $\mathscr{T}$: clearly, the boundary of $\overline{\mathscr{J}_\Lambda}$ consists of reduced tridiagonal matrices with non-negative off-diagonal entries, including the $n!$ diagonal matrices obtained by permuting the eigenvalues $\lambda_1, \ldots, \lambda_n$. The boundary of $\overline{\mathscr{J}_\Lambda}$ is not a smooth manifold: it has a polytope-like cell structure which was described in [19]. We now give a more explicit description.

For $T \in \overline{\mathscr{J}_\Lambda}$, write a diagonalization $T = Q^*\Lambda Q$, $Q \in O(n)$. Consider the matrix $\widehat{T} = Q\Lambda Q^*$: this matrix is not well defined (due to the sign ambiguity in Q) but the diagonal of $\widehat{T}$ is. Define $\iota(T)$ to be the diagonal matrix coinciding with $\widehat{T}$ on the diagonal. Also, let $\mathscr{P}_\Lambda$ be the convex hull of the set of $n!$ matrices Λ^π, $\pi \in S_n$.

Theorem 2.3 [2]. *The map ι constructed above is a homeomorphism $\iota : \overline{\mathscr{J}_\Lambda} \to \mathscr{P}_\Lambda$ which is a smooth diffeomorphism between interiors. Furthermore, $\iota(\Lambda^\pi) = \Lambda^{\pi^{-1}}$.*

The original proof of this theorem uses a result of Atiyah on the convexity of the image of moment maps defined on Kähler manifolds [1]; a more elementary proof is given in [12]. We find this sequence of results to be a good example of the interplay between high and low roads in linear algebra, so eloquently described in [18].

We now present in detail the case $n = 3$, where $\overline{\mathscr{J}_\Lambda}$ and $\mathscr{P}_\Lambda$ have dimension 2. Take $\Lambda = \mathrm{diag}(4, 5, 7)$; $\mathscr{P}_\Lambda$ is a hexagon contained in the plane $x + y + z = 4 + 5 + 7$. The spaces $\overline{\mathscr{J}_\Lambda}$ and $\mathscr{P}_\Lambda$ are given in Fig. 1. The polygon $\mathscr{P}_\Lambda$ is drawn in scale; the drawing of $\overline{\mathscr{J}_\Lambda}$ is schematic.

The triples in the diagram of $\overline{\mathscr{J}_\Lambda}$ are of two kinds. The vertices, which are diagonal matrices, are labelled by the three diagonal entries. The edges have stars in the place of a 2×2 block. Thus, for instance, the edge $(*, *, 7)$ consists of matrices of the form

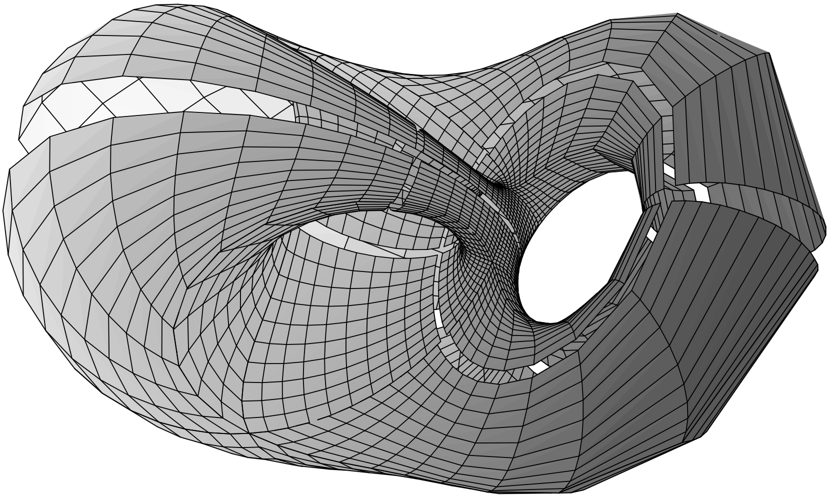

Fig. 2. A 3d rendition of $\mathscr{T}_\Lambda$ for $\Lambda = \mathrm{diag}(4, 5, 7)$.

$$\frac{1}{2}\begin{pmatrix} 9-\cos 2\theta & \sin 2\theta & 0 \\ \sin 2\theta & 9+\cos 2\theta & 0 \\ 0 & 0 & 14 \end{pmatrix} = \begin{pmatrix} c & s & 0 \\ -s & c & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 4 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 7 \end{pmatrix}\begin{pmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

where θ goes from 0 to $\pi/2$, $c = \cos\theta$ and $s = \sin\theta$. Notice that the vertices in $\overline{\mathscr{J}_\Lambda}$ and $\mathscr{P}_\Lambda$ have different adjacencies, in accordance with Theorem 2.3: Λ^{π_1} and Λ^{π_2} are adjacent in $\mathscr{P}_\Lambda$ if and only if $\Lambda^{\pi_1^{-1}}$ and $\Lambda^{\pi_2^{-1}}$ are adjacent in $\overline{\mathscr{J}_\Lambda}$.

Allowing arbitrary signs at off-diagonal entries, we consider the *tridiagonal isospectral manifold* $\mathscr{T}_\Lambda$, the set of real symmetric tridiagonal matrices T which are conjugate to Λ. Define the *sign sequence* of an unreduced matrix T as $\mathrm{signseq}(T) = (\mathrm{sign}(T_{21}), \mathrm{sign}(T_{32}), \ldots, \mathrm{sign}(T_{n,n-1}))$. The subset of $\mathscr{T}_\Lambda$ of unreduced matrices splits into 2^{n-1} connected components according to the sign sequence. Conjugation by sign diagonals takes one component to another. Thus, $\mathscr{T}_\Lambda$ is obtained by gluing 2^{n-1} copies of $\overline{\mathscr{J}_\Lambda}$ along their boundaries.

It is shown in [19] that $\mathscr{T}_\Lambda$ is a compact orientable manifold by proving that simple spectra are regular values of the restriction to $\mathscr{T}$ of the ordered spectrum map σ_o.

For $\Lambda = \mathrm{diag}(4, 5, 7)$, Fig. 2 shows the manifold $\mathscr{T}_\Lambda$, a bitorus. The vector space $\mathscr{T}$ receives an Euclidean metric via the inner product $\langle T_1, T_2\rangle = \mathrm{tr}(T_1T_2)$. The manifold $\mathscr{T}_\Lambda$ is then contained in the intersection of the hyperplane of matrices of trace $4 + 5 + 7$ and the sphere of matrices T with $\langle T, T\rangle = 4^2 + 5^2 + 7^2$: this intersection is isometric to a sphere centered at the origin in $\mathbb{R}^4$. A stereographic projection takes this sphere (and its subset $\mathscr{T}_\Lambda$) to $\mathbb{R}^3$: Fig. 2 is a snapshot of the image of $\mathscr{T}_\Lambda$ under this projection. The small gaps were artificially introduced: these tubular neighborhoods of circles in $\mathbb{R}^3$ split the manifold into the four hexagons $E\overline{\mathscr{J}_\Lambda}E$, $E \in \mathscr{E}$.

Fig. 3 shows again $\mathscr{T}_\Lambda$ for this example in a more schematic fashion. The four hexagons stand for the components of the subset of unreduced matrices: sign sequences label the hexagons. Vertices are diagonal matrices and edges with the same label are identified.

The bitorus is decomposed as a disjoint union of four open hexagons, six open edges and six vertices. We generalize this cell decomposition. Any tridiagonal matrix $T \in \mathscr{T}_\Lambda$ splits into unreduced blocks $T_1, \ldots, T_k$ along the diagonal. Consider the subspectra $\Lambda_i = \mathrm{diag}(\sigma_o(T_i))$ and the sign sequences $\mathrm{signseq}(T_i)$. The (*open*) *cell containing* T is the subset of $\mathscr{T}_\Lambda$ of matrices with

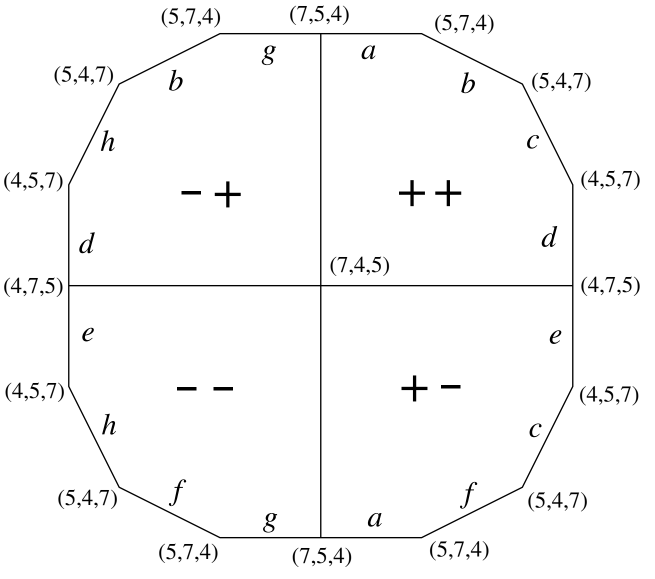

Fig. 3. Gluing instructions for the manifold $\mathscr{T}_\Lambda$.

the same block partition, subspectra and sign sequences as T. The cell containing T is naturally identified with $\mathscr{J}_{\Lambda_1} \times \cdots \times \mathscr{J}_{\Lambda_k}$ and therefore diffeomorphic to $\mathbb{R}^{n-k}$, from Theorem 2.2. The vertices (or cells of dimension 0) of $\mathscr{T}_\Lambda$ are the diagonal matrices Λ^π and the set $\mathscr{J}_\Lambda$ of Jacobi matrices is the cell of maximal dimension $n-1$ defined by $\mathrm{signseq}(T) = (+, +, \ldots, +)$.

The reader should notice that norming constants do not admit a smooth natural extension to $\mathscr{T}_\Lambda$. Indeed, again in Fig. 3, norming constants are positive on the $++$ cell of Jacobi matrices. Crossing the horizontal axis to the cell $+-$ takes the norming constant w_2 (associated with $\lambda_2 = 5$) through 0 so, to guarantee smoothness, we should have signs $+-+$ for the norming constants in the cell $+-$. On the other hand, we can also go from $++$ to $+-$ through the edges a or c and such crossings would induce the sign patterns $-++$ and $++-$, respectively.

3. Bidiagonal coordinates

In this section, we construct an atlas for $\mathscr{T}_\Lambda$ given by a family of charts ψ_π indexed by the permutations $\pi \in S_n$. Each chart is a diffeomorphism $\psi_\pi : \mathscr{U}_\Lambda^\pi \to \mathbb{R}^{n-1}$ and the chart domains $\mathscr{U}_\Lambda^\pi$, centered at the diagonal matrices Λ^π (in the sense that $\psi_\pi(\Lambda^\pi) = 0$), form an open cover of $\mathscr{T}_\Lambda$. The *bidiagonal coordinates* β_i^π for a matrix $T \in \mathscr{U}_\Lambda^\pi$ are the entries of the vector $\psi_\pi(T)$.

For $n = 3$, $\Lambda = \mathrm{diag}(4, 5, 7)$ and π given by $\pi(1) = 3$, $\pi(2) = 1$, $\pi(3) = 2$ so that $\Lambda^\pi = \mathrm{diag}(7, 4, 5)$ the set $\mathscr{U}_\Lambda^\pi$ is the interior of the polygon in Fig. 3. Bidiagonal coordinates were used to produce Fig. 2: $\mathscr{T}_\Lambda$ was partitioned into six quadrilaterals centered at diagonal matrices. This decomposition of $\mathscr{T}_\Lambda$ has four vertices (one in the interior of each of the four hexagons described in the previous section); each quadrilateral touches each vertex once. In the figure, the small gaps split each quadrilateral into four smaller ones; boundaries between quadrilaterals are visible as the lines along which the mesh loses smoothness. Lines in each quadrilateral are level curves of bidiagonal coordinates β_i^π. We first define the chart domains $\mathscr{U}_\Lambda^\pi$.

Definition 3.1. For a permutation π, the *chart domain* $\mathscr{U}_\Lambda^\pi$ is the set of matrices $T \in \mathscr{T}_\Lambda$ admitting a π-normalized diagonalization, i.e., the matrices T for which there exists an LU-positive matrix $Q_\pi \in O(n)$ with $T = Q_\pi^* \Lambda^\pi Q_\pi$.

We now present some properties of the sets $\mathscr{U}_\Lambda^\pi$.

Lemma 3.2. (a) *The sets* $\mathscr{U}_\Lambda^\pi \subset \mathscr{T}_\Lambda$ *form an open cover of* $\mathscr{T}_\Lambda$.

(b) *If* $E \in \mathscr{E}$ *and* $T \in \mathscr{U}_\Lambda^\pi$ *then* $ETE \in \mathscr{U}_\Lambda^\pi$.

(c) *If* $T \in \mathscr{T}_\Lambda$ *is unreduced then* $T \in \mathscr{U}_\Lambda^\pi$ *for all permutations* π. *In particular, each set* $\mathscr{U}_\Lambda^\pi$ *is dense in* $\mathscr{T}_\Lambda$.

(d) *Take* $T \in \mathscr{T}_\Lambda$ *with unreduced blocks* $T_1, \ldots, T_k$ *of dimensions* $n_1, \ldots, n_k$ *along the diagonal. For a permutation* π, *split* Λ^π *in blocks*:

$$(\Lambda^\pi)_i = \operatorname{diag}\left(\lambda^\pi_{n_1+\cdots+n_{i-1}+1}, \ldots, \lambda^\pi_{n_1+\cdots+n_{i-1}+n_i}\right).$$

Then $T \in \mathscr{U}_\Lambda^\pi$ *if and only if* T_i *is conjugate to* $(\Lambda^\pi)_i$ *for* $i = 1, \ldots, k$.

Proof. (a) For $T \in \mathscr{T}_\Lambda$, write $T = Q^*\Lambda Q$ for some $Q \in O(n)$. Write the PLU factorization of Q, i.e., $Q = PLU$ where P is a permutation matrix, L is lower unipotent and U is upper triangular. Notice that this is usually possible for $P = P_\pi$ for several permutations $\pi \in S_n$. Thus, all the leading principal minors of $P_\pi^{-1}Q$ are invertible and there exists $E \in \mathscr{E}$ such that $Q_\pi = EP_\pi^{-1}Q$ is LU-positive and $T = Q^*\Lambda Q = Q_\pi^*\Lambda^\pi Q_\pi$ belongs to $\mathscr{U}_\Lambda^\pi$. The set of LU-positive matrices is open in $\mathbb{R}^{n\times n}$ and therefore each $\mathscr{U}_\Lambda^\pi$ is also open in $\mathscr{T}_\Lambda$.

(b) If $T = Q_\pi^*\Lambda^\pi Q_\pi$ is the π-normalized factorization of $T \in \mathscr{U}_\Lambda^\pi$ then $ETE = (EQ_\pi E)^* \Lambda^\pi (EQ_\pi E)$. The matrix $EQ_\pi E$ is LU-positive and therefore $ETE \in \mathscr{U}_\Lambda^\pi$.

(c) The case where T is a Jacobi matrix is discussed in Theorem 2.2. If T is unreduced then there exists $E \in \mathscr{E}$ such that ETE is Jacobi and item (b) completes the argument.

(d) Consider a permutation π, $T \in \mathscr{T}_\Lambda$ with unreduced blocks $T_1, \ldots, T_k$ and the diagonal blocks $(\Lambda^\pi)_i$ as above. From item (c), if T_i and $(\Lambda^\pi)_i$ are conjugate then there exist LU-positive matrices $Q_i \in O(n_i)$ with $T_i = Q_i^*(\Lambda^\pi)_i Q_i$. Let $\widetilde{Q}$ be the matrix with blocks Q_i: the matrix $\widetilde{Q}$ is LU-positive and orthogonal; $T = (\widetilde{Q})^*\Lambda^\pi\widetilde{Q}$ implies $T \in \mathscr{U}_\Lambda^\pi$.

Conversely, assume that $T \in \mathscr{U}_\Lambda^\pi$ admits a block decomposition. Then $T = (P_\pi LU)^{-1}\Lambda(P_\pi LU)$ yields $UTU^{-1} = L^{-1}\Lambda^\pi L$ and we therefore have $U_iT_iU_i^{-1} = L_i^{-1}(\Lambda^\pi)_i L_i$ where U_i and L_i are blocks along the diagonal for U and L. $\square$

Item (d) yields an alternative description of the chart domain $\mathscr{U}_\Lambda^\pi$: it is the union of all cells in $\mathscr{T}_\Lambda$ whose closure contains Λ^π.

We now construct charts $\psi_\pi : \mathscr{U}_\Lambda^\pi \to \mathbb{R}^{n-1}$ and their inverses ϕ_π.

Definition 3.3. Given $\beta_1^\pi, \ldots, \beta_{n-1}^\pi$ and $\Lambda^\pi = \operatorname{diag}(\lambda_1^\pi, \ldots, \lambda_n^\pi)$ build the bidiagonal matrix

$$B_\pi = \begin{pmatrix} \lambda_1^\pi & & & & \\ \beta_1^\pi & \lambda_2^\pi & & & \\ & \beta_2^\pi & \lambda_3^\pi & & \\ & & \ddots & \ddots & \\ & & & \beta_{n-1}^\pi & \lambda_n^\pi \end{pmatrix}.$$

Take the diagonalization $B_\pi = L_\pi^{-1}\Lambda^\pi L_\pi$ where L_π is lower triangular with unit diagonal. Define the *inverse chart* $\phi_\pi : \mathbb{R}^{n-1} \to \mathscr{U}_\Lambda^\pi$ by

$$\phi_\pi(\beta_1^\pi, \dots, \beta_{n-1}^\pi) = \mathbf{Q}(L_\pi)^* \Lambda^\pi \mathbf{Q}(L_\pi).$$

Notice that $\phi_\pi(0) = \Lambda^\pi$. It is easy to see that a matrix L_π as above exists; an explicit formula for its entries is given in the proof of Proposition 3.6. The claim that $\mathscr{U}_\Lambda^\pi$ is a valid counterdomain for ϕ_π requires a proof. Set $Q_\pi = \mathbf{Q}(L_\pi)$: the matrix $T = \phi_\pi(\beta_1^\pi, \dots, \beta_{n-1}^\pi) = Q_\pi^* \Lambda^\pi Q_\pi$ is clearly symmetric. On the other hand, the factorization $T = \mathbf{R}(L_\pi) B_\pi (\mathbf{R}(L_\pi))^{-1}$ implies that T is upper Hessenberg and therefore $T \in \mathscr{T}_\Lambda$. Since $\mathbf{R}(L_\pi)$ has positive diagonal and $Q_\pi = L_\pi(\mathbf{R}(L_\pi))^{-1}$, we have that the matrix Q_π is LU-positive, $T = Q_\pi^* \Lambda^\pi Q_\pi$ is a π-normalized diagonalization and therefore $T \in \mathscr{U}_\Lambda^\pi$.

Definition 3.4. For $T \in \mathscr{U}_\Lambda^\pi$, take its π-normalized diagonalization $T = Q_\pi^* \Lambda^\pi Q_\pi$ and write $L_\pi = \mathbf{L}(Q_\pi)$, $U_\pi = \mathbf{U}(Q_\pi)$, $R_\pi = U_\pi^{-1}$. Set

$$B_\pi = R_\pi^{-1} T R_\pi = L_\pi^{-1} \Lambda^\pi L_\pi.$$

The matrix B_π is bidiagonal and its off-diagonal entries $\beta_i^\pi = (B_\pi)_{i+1,i}$, $i = 1, \dots, n-1$, are the *π-bidiagonal coordinates* of T. The *chart* $\psi_\pi : \mathscr{U}_\Lambda^\pi \to \mathbb{R}^{n-1}$ is the map taking T to $(\beta_1^\pi, \dots, \beta_{n-1}^\pi)$.

We prove that B_π is indeed bidiagonal. From $B_\pi = R_\pi^{-1} T R_\pi$, B_π is upper Hessenberg and from $B_\pi = L_\pi^{-1}\Lambda^\pi L_\pi$, it is lower triangular with diagonal entries $\lambda_1^\pi, \dots, \lambda_n^\pi$.

The maps ψ_π and ϕ_π are clearly smooth. By construction, one is the inverse of the other, implying the following result.

Theorem 3.5. *The map $\phi_\pi : \mathbb{R}^{n-1} \to \mathscr{U}_\Lambda^\pi$ is a diffeomorphism with inverse $\psi_\pi : \mathscr{U}_\Lambda^\pi \to \mathbb{R}^{n-1}$.*

As an example of bidiagonal coordinates, let $\Lambda = \mathrm{diag}(4, 5, 7)$. Set $\pi(1) = 3$, $\pi(2) = 1$, $\pi(3) = 2$. Matrices will be described by their π-bidiagonal coordinates $x = \beta_1^\pi$ and $y = \beta_2^\pi$. Since $B_\pi = L_\pi^{-1}\Lambda^\pi L_\pi$, we obtain

$$\Lambda^\pi = \begin{pmatrix} 7 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix}, \quad B_\pi = \begin{pmatrix} 7 & 0 & 0 \\ x & 4 & 0 \\ 0 & y & 5 \end{pmatrix}, \quad L_\pi = \begin{pmatrix} 1 & 0 & 0 \\ -x/3 & 1 & 0 \\ -xy/2 & y & 1 \end{pmatrix}$$

and writing $Q_\pi = L_\pi U_\pi$ we have

$$Q_\pi = \frac{1}{r_1 r_2} \begin{pmatrix} 6r_2 & 6x(2+3y^2) & xyr_1 \\ -2xr_2 & 3(12 + x^2y^2) & -6yr_1 \\ -3xyr_2 & 2y(18 - x^2) & 6r_1 \end{pmatrix},$$

where $r_1 = \sqrt{36 + 4x^2 + 9x^2y^2}$ and $r_2 = \sqrt{36 + 36y^2 + x^2y^2}$. From $T = Q_\pi^* \Lambda^\pi Q_\pi$, we have $T = \Lambda^\pi + M/(r_1^2 r_2^2)$ where

$$M = \begin{pmatrix} -6x^2(2+3y^2)r_2^2 & 6xr_2^3 & 0 \\ 6xr_2^3 & (72 + 108y^2)r_1^2 - (72 - 4x^2)r_2^2 & 6yr_1^3 \\ 0 & 6yr_1^3 & -2y^2(18 - x^2)r_1^2 \end{pmatrix}.$$

This is an explicit parametrization $\phi_\pi : \mathbb{R}^2 \to \mathscr{U}_\Lambda^\pi \subset \mathscr{T}_\Lambda$ of the polygon in Fig. 3. From this formula, $x = 0$ implies $(T)_{11} = 7$ and $(T)_{21} = 0$ while $y = 0$ gives $(T)_{33} = 5, (T)_{32} = 0$, consistent with the description of $\mathscr{U}_\Lambda^\pi$ in Lemma 3.2.

Proposition 3.6. *For any permutation π and any Jacobi matrix $J \in \mathscr{J}_\Lambda$, the norming constants w_i and the π-bidiagonal coordinates β_i^π are related by*

$$w_{\pi(i)} = w_{\pi(1)} \left| \frac{\beta_1^\pi \cdots \beta_{i-1}^\pi}{(\lambda_i^\pi - \lambda_1^\pi) \cdots (\lambda_i^\pi - \lambda_{i-1}^\pi)} \right|, \quad 2 \leqslant i \leqslant n,$$

$$\beta_i^\pi = \left| \frac{(\lambda_{\pi(i+1)} - \lambda_{\pi(1)}) \cdots (\lambda_{\pi(i+1)} - \lambda_{\pi(i)})}{(\lambda_{\pi(i)} - \lambda_{\pi(1)}) \cdots (\lambda_{\pi(i)} - \lambda_{\pi(i-1)})} \right| \frac{w_{\pi(i+1)}}{w_{\pi(i)}}, \quad 1 \leqslant i \leqslant n-1.$$

Proof. Let Λ^π and B_π be as above. Set

$$L = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \frac{\beta_1^\pi}{\lambda_2^\pi - \lambda_1^\pi} & 1 & 0 & \cdots & 0 \\ \frac{\beta_1^\pi \beta_2^\pi}{(\lambda_3^\pi - \lambda_1^\pi)(\lambda_3^\pi - \lambda_2^\pi)} & \frac{\beta_2^\pi}{\lambda_3^\pi - \lambda_2^\pi} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ \frac{\beta_1^\pi \beta_2^\pi \cdots \beta_{n-1}^\pi}{(\lambda_n^\pi - \lambda_1^\pi)(\lambda_n^\pi - \lambda_2^\pi) \cdots (\lambda_n^\pi - \lambda_{n-1}^\pi)} & \frac{\beta_2^\pi \cdots \beta_{n-1}^\pi}{(\lambda_n^\pi - \lambda_2^\pi) \cdots (\lambda_n^\pi - \lambda_{n-1}^\pi)} & & \cdots & 1 \end{pmatrix}.$$

A straightforward computation verifies that $LB_\pi = \Lambda^\pi L$ and therefore $L = L_\pi$.

Norming constants are given by the absolute values of entries in the first column of Q_π which in turn is the normalization of the first column of L_π. $\square$

Bidiagonal coordinates change signs together with off-diagonal entries in a simple fashion.

Lemma 3.7. *If $E = \mathrm{diag}(\sigma_1, \ldots, \sigma_n) \in \mathscr{E}, T \in \mathscr{U}_\Lambda^\pi$, and $\psi_\pi(T) = (\beta_1^\pi, \ldots, \beta_{n-1}^\pi)$ then $\psi_\pi(ETE) = (\sigma_1\sigma_2\beta_1^\pi, \ldots, \sigma_{n-1}\sigma_n\beta_{n-1}^\pi)$. In other words, if B_π and $\widetilde{B}_\pi$ are the bidiagonal matrices associated to T and ETE (as in Definition 3.4), respectively, then $\widetilde{B}_\pi = EB_\pi E$.*

Proof. From Lemma 3.2, if $T \in \mathscr{U}_\Lambda^\pi$ then $\widetilde{T} = ETE \in \mathscr{U}_\Lambda^\pi$. Clearly, if the π-normalized decomposition of T is $T = Q_\pi^* \Lambda^\pi Q_\pi$ then $ETE = (EQ_\pi E)^* \Lambda^\pi (EQ_\pi E)$ is the π-normalized diagonalization of ETE. Also, $\mathbf{L}(EQ_\pi E) = E\mathbf{L}(Q_\pi)E$ and therefore, if $L_\pi = \mathbf{L}(Q_\pi)$ then $\widetilde{B}_\pi = (EL_\pi E)^{-1} \Lambda^\pi (EL_\pi E) = EB_\pi E$. $\square$

Norming constants break down at the boundary of $\overline{\mathscr{J}_\Lambda}$. We will prove in the following proposition, however, that near a reduced matrix T with $(T)_{i+1,i} = 0$ the values of $(T)_{i+1,i}$ and β_i^π are comparable. This will be useful when we use bidiagonal coordinates to study the asymptotics of isospectral maps.

Proposition 3.8. *Given Λ and π, the quotient $q_i^\pi : \mathscr{U}_\Lambda^\pi \to \mathbb{R}$ defined by $q_i^\pi(T) = \beta_i^\pi(T)/((T)_{i+1,i})$ is smooth, positive and $q_i^\pi(\Lambda^\pi) = 1$. Also, $q_i^\pi(ETE) = q_i^\pi(T)$ for all $T \in \mathscr{U}_\Lambda^\pi$ and $E \in \mathscr{E}$.*

In particular β_i^π and $(T)_{i+1,i}$ have the same sign regardless of π.

Proof. Clearly, $(T)_{i+1,i} = 0$ if and only if $ETE = T$ where $E_{j,j} = 1$ (resp. -1) for $j \leqslant i$ (resp. $j \geqslant i+1$). Thus, from Lemma 3.7, $\beta_i^\pi(T) = 0$ if and only if $(T)_{i+1,i} = 0$.

We study the i-th partial derivative of $(\phi_\pi(\beta_1^\pi, \dots, \beta_{n-1}^\pi))_{i+1,i}$ when $\beta_i^\pi = 0$. Take a path $T : \mathbb{R} \to \mathscr{T}_\Lambda$, $T(t) = \phi_\pi(\beta_1^\pi, \dots, t, \dots, \beta_{n-1}^\pi)$. From Lemma 3.7, all entries of $T(t)$ except $(i+1, i)$ (and $(i, i+1)$) are even functions of t and therefore the corresponding entries of $T'(0)$ equal 0. On the other hand, since ϕ_π is a diffeomorphism, $T'(0)$ must be nonzero. It follows that $(T'(0))_{i+1,i} \neq 0$ and therefore $q_i^\pi(T)$ is well defined, smooth and nonzero even when the denominator vanishes, i.e., at reduced matrices.

The symmetry property indicated in the last claim follows from Lemma 3.7. Positivity is obvious for Jacobi matrices, extends to unreduced matrices by symmetry and to reduced matrices by continuity. In order to compute $q_i^\pi(\Lambda^\pi)$, consider the path $T(t) = \phi_\pi(0, \dots, t, \dots, 0)$ (with t in the i-th position). Clearly, $B_\pi(t) = \Lambda^\pi + t(e_{i+1})^* e_i$ so that $\beta_i^\pi(t) = t$. A straightforward computation yields

$$(T(t))_{i+1,i} = \frac{(\lambda_{i+1}^\pi - \lambda_i^\pi)^2}{(\lambda_{i+1}^\pi - \lambda_i^\pi)^2 + t^2} t; \quad q_i^\pi(T(t)) = \frac{(\lambda_{i+1}^\pi - \lambda_i^\pi)^2 + t^2}{(\lambda_{i+1}^\pi - \lambda_i^\pi)^2}.$$

The result now follows by setting $t = 0$. $\square$

4. Iterations in $\mathscr{U}_\Lambda^\pi$

We now apply bidiagonal coordinates to the study of the dynamics of QR type iterations. As a simple example, we present in Theorem 4.2 a new proof of the well known fact that the Rayleigh quotient shift iteration has cubic convergence. A subtler example is the Wilkinson's shift iteration which is studied with the same technique in [10,11]. Excellent references for the spectral theory of Jacobi matrices are [5,8,14].

For an open neighborhood $X \subset \mathbb{R}$ of the spectrum $\{\lambda_1, \dots, \lambda_n\} = \sigma(\Lambda)$ and a continuous function $f : X \to \mathbb{R}$ taking nonzero values on $\sigma(\Lambda)$, there is a smooth map $F : \mathscr{T}_\Lambda \to \mathscr{T}_\Lambda$, the *$QR$ step induced by f*, given by

$$F(T) = \mathbf{Q}(f(T))^* T \mathbf{Q}(f(T)).$$

Continuity of f is sufficient to imply that F is a well defined smooth function: indeed, if f and the polynomial p coincide on $\sigma(\Lambda)$ then $f(T) = p(T)$ for all $T \in \mathscr{T}_\Lambda$ and therefore $F = P$, the QR step induced by p.

The standard QR step corresponds to $f(x) = x$. Since T and $f(T)$ commute, we also have

$$F(T) = \mathbf{R}(f(T)) T \mathbf{R}(f(T))^{-1}.$$

From the first formula, $F(T)$ is symmetric; from the second, it is upper Hessenberg with subdiagonal elements with the same signs as in T. Thus, $F : \mathscr{T}_\Lambda \to \mathscr{T}_\Lambda$ preserves $\mathscr{J}_\Lambda$, the other cells and the open subsets $\mathscr{U}_\Lambda^\pi$.

Let $F^{\phi_\pi} = \phi_\pi^{-1} \circ F \circ \phi_\pi : \mathbb{R}^{n-1} \to \mathbb{R}^{n-1}$; in other words, F^{ϕ_π} is obtained from $F|_{\mathscr{U}_\Lambda^\pi}$ by a change of variables using bidiagonal coordinates.

Proposition 4.1. *For f taking nonzero values on the spectrum of T,*

$$F^{\phi_\pi}(\beta_1^\pi, \dots, \beta_{n-1}^\pi) = \left(\left| \frac{f(\lambda_{\pi(2)})}{f(\lambda_{\pi(1)})} \right| \beta_1^\pi, \dots, \left| \frac{f(\lambda_{\pi(n)})}{f(\lambda_{\pi(n-1)})} \right| \beta_{n-1}^\pi \right).$$

Also, QR iterations generically converge to diagonal matrices. More precisely, if $T \in \mathscr{U}_\Lambda^\pi$ and $|f(\lambda_{\pi(1)})| > |f(\lambda_{\pi(2)})| > \cdots > |f(\lambda_{\pi(n)})|$, then $\lim_{k\to+\infty} F^k(T) = \Lambda^\pi$ with asymptotics

$$\beta_i^\pi = \lim_{k\to+\infty} (F^k(T))_{i+1,i} \left|\frac{f(\lambda_{\pi(i)})}{f(\lambda_{\pi(i+1)})}\right|^k.$$

Proof. Take $T \in \mathscr{U}_\Lambda^\pi$ and set $T' = F(T) = \mathbf{Q}(f(T))^* T \mathbf{Q}(f(T))$. We show that $T' \in \mathscr{U}_\Lambda^\pi$ and relate the corresponding matrices B_π and B'_π. Consider the π-normalized diagonalization $T = Q_\pi^* \Lambda^\pi Q_\pi$ and write $L_\pi = \mathbf{L}(Q_\pi)$. Since $f(T) = Q_\pi^* f(\Lambda^\pi) Q_\pi$ and $\mathbf{Q}(ZM) = Z\mathbf{Q}(M)$ for an arbitrary matrix $Z \in O(n)$ and invertible M, we have $T' = (\widetilde{Q})^* \Lambda^\pi \widetilde{Q}$ where $\widetilde{Q} = Q_\pi \mathbf{Q}(Q_\pi^* f(\Lambda^\pi) Q_\pi) = \mathbf{Q}(f(\Lambda^\pi) Q_\pi)$. Take $Q'_\pi = \mathbf{Q}(|f|(\Lambda^\pi) Q_\pi)$: clearly, Q'_π is LU-positive and $Q'_\pi = E\widetilde{Q}$ for some $E \in \mathscr{E}$ and therefore $T' = (Q'_\pi)^* \Lambda^\pi Q'_\pi$ is the π-normalized diagonalization of $T' \in \mathscr{U}_\Lambda^\pi$. Write $L_\pi = \mathbf{L}(Q_\pi)$, $L'_\pi = \mathbf{L}(Q'_\pi)$. Since $\mathbf{L}(M) = \mathbf{L}(MR)$ for arbitrary LU-positive matrices M and invertible, upper triangular R, we have $\mathbf{L}(M) = \mathbf{L}(\mathbf{Q}(M))$ and thus $L'_\pi = \mathbf{L}(|f|(\Lambda^\pi) Q_\pi)$. Notice that if D is an invertible diagonal matrix and M is LU-positive then $\mathbf{L}(DM) = D\mathbf{L}(M)D^{-1}$: we obtain $L'_\pi = |f|(\Lambda^\pi) L_\pi (|f|(\Lambda^\pi))^{-1}$ and therefore

$$B'_\pi = (L'_\pi)^{-1} \Lambda^\pi L_\pi = (|f|(\Lambda^\pi)) B_\pi (|f|(\Lambda^\pi))^{-1}.$$

This finishes the proof of the first formula. The convergence properties now follow easily from Proposition 3.8. □

This proposition yields yet another evidence for the naturality of the bidiagonal coordinates β_i^π.

The cubic convergence to deflation of the QR iteration with Rayleigh quotient shift is well known [14]; using bidiagonal coordinates, we deduce it from a Taylor expansion. For $s \in \mathbb{R}$, let $f_s(x) = x - s$ so that the QR step $F_s : \mathscr{T}_\Lambda \to \mathscr{T}_\Lambda$ is defined for $s \notin \sigma(\Lambda)$. In other words, we have a map $\mathbf{F} : (\mathbb{R} \setminus \sigma(\Lambda)) \times \mathscr{T}_\Lambda \to \mathscr{T}_\Lambda$, $\mathbf{F}(s, T) = F_s(T)$. The map $\mathbf{F}$ cannot be continuously extended to $\mathbb{R} \times \mathscr{T}_\Lambda$; it follows from Proposition 4.1, however, that $\mathbf{F}$ can be continuously extended to pairs (s, T) if $s = \lambda_i$ and the (possibly reduced) matrix T has the eigenvalue λ_i in the spectrum of its bottom block. More formally, consider the set

$$\mathscr{D}_\mathbf{F} = ((\mathbb{R} \setminus \sigma(\Lambda)) \times \mathscr{T}_\Lambda) \cup \bigcup_{i=1}^n \left(\{\lambda_i\} \times \bigcup_{\pi \in S_n, \pi(i) = n} \mathscr{U}_\Lambda^\pi \right) \subset \mathbb{R} \times \mathscr{T}_\Lambda.$$

The set $\mathscr{D}_\mathbf{F}$ is open since points $T \in \{\lambda_{\pi(n)}\} \times \mathscr{U}_\Lambda^\pi$ admit the explicit open neighborhood $(\lambda_n^\pi - \gamma/2, \lambda_n^\pi + \gamma/2) \times \mathscr{U}_\Lambda^\pi \subset \mathscr{D}_\mathbf{F}$ where $\gamma = \min_{i\neq j} |\lambda_i - \lambda_j|$ is the spectral gap of Λ. The function $\mathbf{F}$ is defined in $\mathscr{D}_\mathbf{F}$ by

$$\mathbf{F}(s, \phi_\pi(\beta_1^\pi, \ldots, \beta_{n-1}^\pi)) = \phi_\pi \left(\left|\frac{\lambda_2^\pi - s}{\lambda_1^\pi - s}\right| \beta_1^\pi, \ldots, \left|\frac{\lambda_n^\pi - s}{\lambda_{n-1}^\pi - s}\right| \beta_{n-1}^\pi \right). \qquad (*)$$

The *QR iteration with Rayleigh quotient shift* $G : \mathscr{D}_G \to \mathscr{T}_\Lambda$ is defined by $G(T) = \mathbf{F}((T)_{n,n}, T)$ where $\mathscr{D}_G \subseteq \mathscr{T}_\Lambda$ is the open set $\{T \in \mathscr{T}_\Lambda | ((T)_{n,n}, T) \in \mathscr{D}_\mathbf{F}\}$. Notice that, from a numerical point of view, falling outside $\mathscr{D}_G$ is an instant win: $(T)_{n,n}$ is an eigenvalue.

The *deflation set* $\Delta_0 \subset \mathscr{T}_\Lambda$ is the set of matrices T with $(T)_{n,n-1} = 0$. The set Δ_0 is the disjoint union of the subsets Δ_0^i of matrices $T \in \Delta_0$ with $(T)_{n,n} = \lambda_i$. Notice that Δ_0^i is diffeomorphic to $\mathscr{T}_{\Lambda_{\hat{i}}}$ where $\Lambda_{\hat{i}} = \mathrm{diag}(\lambda_1, \ldots, \lambda_{i-1}, \lambda_{i+1}, \ldots, \lambda_n)$ and therefore a connected component of Δ_0. Clearly, $\Delta_0 \subset \mathscr{D}_G$ since $T_{n,n-1} = 0$ and $T_{n,n} = \lambda_n^\pi$ imply that $T \in \mathscr{U}_\Lambda^\pi$. The (*compact*) *deflation neighborhood* Δ_ϵ is the set of matrices $T \in \mathscr{T}_\Lambda$ with $|(T)_{n,n-1}| \leqslant \epsilon$.

Theorem 4.2. *There exist $\epsilon > 0$ and $c > 0$ such that $\Delta_\epsilon \subset \mathscr{D}_G$, $G(\Delta_\epsilon) \subset \Delta_\epsilon$ and for all $T \in \Delta_\epsilon$ we have $|(G(T))_{n,n-1}| \leqslant c|(T)_{n,n-1}|^3$.*

Proof. Since the chart domains $\mathscr{U}^\pi_\Lambda$ are open dense sets covering $\mathscr{T}_\Lambda$, there exist compact sets $K_\pi \subset \mathscr{U}^\pi_\Lambda$ with $\bigcup_{\pi \in S_n} K_\pi = \mathscr{T}_\Lambda$. Take $M_\pi > 0$ such that $\psi_\pi(K_\pi)$ is contained in the box $(-M_\pi, M_\pi)^{n-1}$: we then have

$$\Delta_0 = \bigcup_{\pi \in S_n} \phi_\pi((-M_\pi, M_\pi)^{n-2} \times \{0\}).$$

Equation $(*)$ above yields a formula for $G^{\phi_\pi} : \mathscr{D}_{G^{\phi_\pi}} \to \mathbb{R}^{n-1}$ where $\mathscr{D}_{G^{\phi_\pi}} = \psi_\pi(\mathscr{D}_G \cap \mathscr{U}^\pi_\Lambda) \subseteq \mathbb{R}^{n-1}$ is an open set with $\mathbb{R}^{n-2} \times \{0\} \subset \mathscr{D}_{G^{\phi_\pi}}$ and

$$s = s(\beta^\pi_1, \ldots, \beta^\pi_{n-1}) = (\phi_\pi(\beta^\pi_1, \ldots, \beta^\pi_{n-1}))_{n,n}.$$

For each π there exist $\epsilon'_\pi > 0$ such that, if $A'_\pi = (-M_\pi, M_\pi)^{n-2} \times (-\epsilon'_\pi, \epsilon'_\pi)$ then $(\beta^\pi_1, \ldots, \beta^\pi_{n-1}) \in A'_\pi$ implies $|s - \lambda^\pi_n| < \gamma/2$ (where γ is the spectral gap) and therefore $\overline{A'_\pi} \subset \mathscr{D}_{G^{\phi_\pi}}$. Due to the presence of absolute values, the function G^{ϕ_π} is almost certainly not smooth in A'. Set $g_\pi : A'_\pi \to \mathbb{R}$,

$$g_\pi(\beta^\pi_1, \ldots, \beta^\pi_{n-1}) = \frac{\lambda^\pi_n - s}{|\lambda^\pi_{n-1} - s|}.$$

The function g_π is smooth and $\beta^\pi_{n-1} = 0$ implies $g_\pi(\beta^\pi_1, \ldots, \beta^\pi_{n-1}) = 0$. Since g is even (from Lemma 3.7), its first order partial derivatives at points with $\beta^\pi_{n-1} = 0$ all vanish and the Taylor expansion for g_π at such points starts with terms of degree 2. By compactness of $\overline{A'_\pi}$, there exists a constant c_π such that

$$g_\pi(\beta^\pi_1, \ldots, \beta^\pi_{n-1}) \leqslant c_\pi(\beta^\pi_{n-1})^2, \quad |(G^{\phi_\pi}(\beta^\pi_1, \ldots, \beta^\pi_{n-1}))_{n-1}| \leqslant c_\pi|\beta^\pi_{n-1}|^3.$$

From Proposition 3.8, β^π_{n-1} and $(T)_{n,n-1}$ are comparable: there exists $\tilde{c}_\pi$ such that $T \in \phi_\pi(A'_\pi)$ implies

$$|(G(T))_{n,n-1}| \leqslant \tilde{c}_\pi|T_{n,n-1}|^3.$$

Take $c = \max_{\pi \in S_n} \tilde{c}_\pi$ and $\epsilon > 0$ such that $\epsilon < c^{-1/2}$ and $\Delta_\epsilon \subset A'$. If $T \in \Delta_\epsilon$ we therefore have $|(G(T))_{n,n-1}| \leqslant c|(T)_{n,n-1}|^3 \leqslant \epsilon$, proving the claims. □

5. Toda flows

Recall that the Toda flow [6,13,4] solves the differential equation

$$J'(t) = [J(t), \Pi_a(J(t))], \quad J(0) = J_0.$$

Here the bracket is the usual Lie bracket on matrices $[A_1, A_2] = A_1A_2 - A_2A_1$ and $\Pi_a(M)$ is the skew-symmetric matrix having the same lower triangular entries as M. As is well known, this flow preserves spectrum and the set $\overline{\mathscr{J}_\Lambda}$. If $w(t)$ is the vector of norming constants for $J(t)$, we have

$$w(t) = \frac{\exp(t\Lambda)w(0)}{||\exp(t\Lambda)w(0)||}:$$

thus, up to normalization, the function w is the solution of a linear differential equation. Taking quotients and using Proposition 3.6 shows that the evolution of β^π_i is truly linear:

$$\frac{d}{dt}\beta_i^\pi(t) = (\lambda_{\pi(i+1)} - \lambda_{\pi(i)})\beta_i^\pi(t).$$

In other words, $B'_\pi = [B_\pi, -\Lambda^\pi]$.

Clearly, the Toda flow is well defined in $\mathscr{T}_\Lambda$. Similar formulae hold for other flows in the Toda hierarchy: for a function g, consider the differential equation $T' = [T, \Pi_a g(T)]$; it turns out that, despite $g(T)$ not being tridiagonal, $[T, \Pi_a g(T)]$ is symmetric and tridiagonal. Integrate the differential equation to define $T(t)$ for all $t \in \mathbb{R}$. In bidiagonal coordinates, it is easy to compute limits and asymptotics of Toda flows.

Proposition 5.1. *In π-bidiagonal coordinates, the equation $T' = [T, \Pi_a g(T)]$ becomes a decoupled linear system: $\frac{\mathrm{d}}{\mathrm{d}t}\beta_i^\pi = (g(\lambda_{i+1}^\pi) - g(\lambda_i^\pi))\beta_i^\pi$. In particular, if $T(0) \in \mathscr{U}_\Lambda^\pi$ and $g(\lambda_{\pi(1)}) > g(\lambda_{\pi(2)}) > \cdots > g(\lambda_{\pi(n)})$ then $\lim_{t\to+\infty}\beta_k^\pi(t) = 0$, so that $\lim_{t\to+\infty} T(t) = \Lambda^\pi$ with asymptotics*

$$\beta_k^\pi(0) = \lim_{t\to+\infty}(T(t))_{k,k+1}\exp((g(\lambda_{\pi(k)}) - g(\lambda_{\pi(k+1)}))t).$$

Proof. The formula below follows by direct computation [9,12,15,16]:

$$T(t) = \mathbf{Q}(\exp(tg(T(0))))^* T(0)\mathbf{Q}(\exp(tg(T(0)))),$$

or, in other words, $\tau(t) = F(T(0))$ where $f(x) = \exp(tg(x))$. From Proposition 4.1,

$$(\beta_1^\pi(t), \ldots, \beta_{n-1}^\pi(t)) = (e^{(g(\lambda_2^\pi)-g(\lambda_1^\pi))t}\beta_1^\pi(0), \ldots, e^{(g(\lambda_n^\pi)-g(\lambda_{n-1}^\pi))t}\beta_{n-1}^\pi(0))$$

and the differential equation for β_i^π follows by taking derivatives. The last formula is now a consequence of Proposition 3.8. □

As an application of the bidiagonal variables we consider the scattering properties of the Toda flow. From a more physical point of view, the Toda flow is the evolution of n particles of mass 1 on the line given by the Hamiltonian

$$H(x, y) = \sum_{k=1}^n \frac{y_k^2}{2} + \sum_{k=1}^{n-1}\exp(x_k - x_{k+1}),$$

where $x = (x_1, \ldots, x_n)$ and $y = (y_1, \ldots, y_n)$ are respectively the positions and velocities of the particles. Without loss of generality,

$$\sum_k x_k(t) = \sum_k y_k(t) = 0.$$

More explicitly, positions and velocities satisfy the differential equation

$$x'_k = H_{y_k} = y_k, \quad y'_k = -H_{x_k} = \exp(x_{k-1} - x_k) - \exp(x_k - x_{k+1}), \quad k = 1, \ldots, n,$$

where we take the formal boundary conditions $x_0 = -\infty$, $x_{n+1} = \infty$. The two versions of the Toda flow are related by Flaschka's transformation [6]:

$$J_{k,k} = -\frac{1}{2}y_k, \quad J_{k,k+1} = \frac{1}{2}\exp\left(\frac{x_k - x_{k+1}}{2}\right).$$

Notice that $\mathrm{tr}(J) = 0$ for the Jacobi matrix J constructed from x and y.

We know that $J(t)$ tends to $\Lambda^{\pi\pm}$ when $t \to \pm\infty$ where π^- is the identity permutation and π^+ is the reversal $\pi^+(k) = n + 1 - k$. The convergence of the diagonal entries implies that the velocities $y_k(t)$ approach $-2\lambda_{\pi_\pm(k)}$. From the convergence to 0 of the off-diagonal entries, the force $\pm\exp(x_k - x_{k+1})$ between particles k and $k+1$ tends to 0 when $t \to \pm\infty$. Thus, asymptotically, the particles undertake independent uniform motions of the form $x_k(t) \approx c_k^\pm t + d_k^\pm$ when $t \to \pm\infty$. Clearly, $c_k^\pm = -2\lambda_{\pi_\pm(k)}$. The *wave* and *scattering maps* are

$$W^\pm(x_1(0), \ldots, x_n(0), y_1(0), \ldots, y_n(0)) = (c_1^\pm, \ldots, c_n^\pm, d_1^\pm, \ldots, d_n^\pm),$$
$$S(c_1^-, \ldots, c_n^-, d_1^-, \ldots, d_n^-) = (c_1^+, \ldots, c_n^+, d_1^+, \ldots, d_n^+),$$

respectively. They are related by $S \circ W^- = W^+$. Moser [13] proved that S is indeed well defined and computed it. We obtain Moser's result by first computing wave maps in bidiagonal coordinates.

Proposition 5.2. *Given initial conditions* $(x_1(0), \ldots, x_n(0), y_1(0), \ldots, y_n(0))$ *with* $\sum x_k(0) = \sum y_k(0) = 0$, *apply Flaschka's transformation to obtain* $J(0)$ *with eigenvalues* $\lambda_1 < \cdots < \lambda_n$ *and bidiagonal coordinates* $\beta_k^{\pi_\pm}$ *for* $\pi_-(k) = k$ *and* $\pi_+(k) = n+1-k$. *Then*

$$c_k^\pm = -2\lambda_{\pi_\pm(k)}, \quad d_k^\pm = \sum_{j<k} \frac{-2j}{n} \tilde{\beta}_j^{\pi_\pm} + \sum_{j \geqslant k} \frac{2(n-j)}{n} \tilde{\beta}_j^{\pi_\pm} + (n-2k+1)\log 2,$$

where $\tilde{\beta}_k^{\pi_\pm} = \log \beta_k^{\pi_\pm}$. *The scattering map is given by*

$$c_{n+1-k}^+ = c_k^-, \quad d_{n+1-k}^+ = d_k^- + 2\sum_{j<k} \log|c_j^- - c_k^-| - 2\sum_{j>k} \log|c_j^- - c_k^-|.$$

Proof. From Proposition 5.1 with $g(z) = z$,

$$J_{k,k+1} = \frac{1}{2}\exp\left(\frac{x_k - x_{k+1}}{2}\right) \approx \exp((\lambda_{\pi_\pm(k+1)} - \lambda_{\pi_\pm(k)})t)\beta_k^{\pi_\pm}$$

in the sense that quotients tend to 1 when $t \to \pm\infty$. Taking logs,

$$(x_k - x_{k+1}) - 2(\lambda_{\pi_\pm(k+1)} - \lambda_{\pi_\pm(k)})t \approx (d_k^\pm - d_{k+1}^\pm) = 2\tilde{\beta}_k^{\pi_\pm} + 2\log 2,$$

where now the difference goes to zero. Since $\sum_k x_k = 0$, we have $\sum_k d_k^\pm = 0$ and the formula for the wave operator follows.

Proposition 3.6 yields $\tilde{\beta}_k^+ = -\tilde{\beta}_{n-k}^- + \delta_k$ where

$$\delta_k = \left(\sum_{j>n-k} \epsilon_{n-k,j} - \sum_{j<n-k} \epsilon_{n-k,j}\right) - \left(\sum_{j>n+1-k} \epsilon_{n+1-k,j} - \sum_{j<n+1-k} \epsilon_{n+1-k,j}\right)$$

and $\epsilon_{ij} = \log|\lambda_{\pi^-(i)} - \lambda_{\pi^-(j)}|$. Use this equation to write

$$\begin{aligned} d_k^+ = &-\left(\sum_{j<k} \frac{-2j}{n} \tilde{\beta}_{n-j}^- + \sum_{j \geqslant k} \frac{2(n-j)}{n} \tilde{\beta}_{n-j}^-\right) \\ &+ \sum_{j<k} \frac{-2j}{n} \delta_j + \sum_{j \geqslant k} \frac{2(n-j)}{n} \delta_j + (n-2k+1)\log 2. \end{aligned}$$

Replacing k by $r(k) = n+1-k$ in the equation for d_k^- yields

$$d_{n+1-k}^- = -\left(\sum_{j<k} \frac{-2j}{n} \tilde{\beta}_{n-j}^- + \sum_{j \geqslant k} \frac{2(n-j)}{n} \tilde{\beta}_{n-j}^-\right) - (n-2k+1)\log 2$$

and therefore

$$d_k^+ = d_{n+1-k}^- + \sum_{j<k} \frac{-2j}{n}\delta_j + \sum_{j\geqslant k} \frac{2(n-j)}{n}\delta_j + 2(n-2k+1)\log 2.$$

The simplification yielding the scattering map is now an easy exercise. □

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