Identities and exponential bounds for transfer matrices

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Abstract. This paper is about analytic properties of single transfer matrices originating from general block-tridiagonal or banded matrices. Such matrices occur in various applications in physics and numerical analysis. The eigenvalues of the transfer matrix describe localization of eigenstates and are linked to the spectrum of the block tridiagonal matrix by a determinantal identity. If the block tridiagonal matrix is invertible, it is shown that half of the singular values of the transfer matrix have a lower bound exponentially large in the length of the chain, and the other half have an upper bound that is exponentially small. This is a consequence of a theorem by Demko, Moss and Smith on the decay of matrix elements of inverse of banded matrices.

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1. Introduction

Several analytic statements can be made, with minimal hypothesis, on the eigenvalues and the singular values of the transfer matrix that originates from a block tridiagonal matrix, just because of the structure. The same can be said for the eigenvalues of the block matrix itself, and their motion as a parameter changes, that describes the boundary conditions of the chain to which the matrix is related. A brief review is presented, and new results will be given.

Consider the difference equation

$$C_k u_{k-1} + A_k u_k + B_k u_{k+1} = E u_k\,, \qquad k = 1 \dots n, \tag{1}$$

where A_k, B_k, $C_k \in \mathbb{C}^{m\times m}$ are complex non singular square matrices, E is a complex parameter, and $u_k \in \mathbb{C}^m$ are unknown vectors. It is the prototype of several equations that occur in physics or numerical analysis: it may be viewed as a model for a chain of "atoms" or slices of some compound system, with nearest neighbor couplings.
At each k the equation provides u_{k+1} in terms of u_k and u_{k-1}; the recursion is made single-term by doubling the vector and introducing the 1-step transfer matrix $t_k(E)$, of size $2m$:

$$\begin{bmatrix} u_{k+1} \\ u_k \end{bmatrix} = \begin{bmatrix} B_k^{-1}(E - A_k) & -B_k^{-1} C_k \\ \mathbb{I}_m & 0 \end{bmatrix} \begin{bmatrix} u_k \\ u_{k-1} \end{bmatrix}. \tag{2}$$

Iteration builds up the n-step transfer matrix $T(E) = t_n(E)\cdots t_1(E)$ that connects vectors n steps apart:

$$T(E) \begin{bmatrix} u_1 \\ u_0 \end{bmatrix} = \begin{bmatrix} u_{n+1} \\ u_n \end{bmatrix}. \tag{3}$$

One is often interested in the singular values $\sigma_1 \ge \ldots \ge \sigma_{2m}$ of $T(E)$ (the eigenvalues of the positive matrix $(T^\dagger T)^{1/2}$), which describe the growth or decay of $\|u_n\|$. The product of the p largest ones ($p = 1, \ldots, 2m$) can be obtained by the formula $\sigma_1 \cdots \sigma_p = \|\Lambda^p T(E)\|$, where $(\Lambda^p T)(v_1 \wedge \ldots \wedge v_p) =: Tv_1 \wedge \ldots \wedge Tv_p$ extends the action of T to antisymmetric $p-$forms and $\|O\|$ is the sup norm of operators [1, 2]. For real transfer matrices the product has the simple geometric interpretation

$$\sigma_1 \cdots \sigma_p = \sup_{v_1 \ldots v_p} \frac{\text{Volume P}\{Tv_1, \ldots, Tv_p\}}{\text{Volume P}\{v_1, \ldots, v_p\}} \tag{4}$$

where $\text{P}\{v_1, \ldots, v_p\}$ is the parallelogram with sides $v_i \in \mathbb{R}^{2m}$.
When the transfer matrix is the product of random matrices, Oseledets' Multiplicative Ergodic Theorem ensures that (up to a set of realizations of null probability measure) the singular values grow or decay exponentially in n with rates (Lyapunov exponents) $\lambda_k = \lim_{n\to\infty} \frac{1}{n} \ln \sigma_k$ that are independent of the realization [3, 4]. Then:

$$\lambda_1 + \ldots + \lambda_p = \lim_{n\to\infty} \frac{1}{n} \ln \|\Lambda^p T\|.$$

The formula can be implemented numerically for the evaluation of Lyapunov spectra [5]. In the simplectic case ($\lambda_{m+k} = -\lambda_k$) the average of the positive Lyapunov exponents is expressible in terms of the average distribution of eigenvalues of the Hermitian random matrices associated to (1):

$$\frac{\lambda_1 + \ldots + \lambda_m}{m} = \int dE' \rho(E') \ln |E - E'| + \text{const.} \tag{5}$$

The formula was obtained by Herbert, Jones and Thouless for $m = 1$, and by Kunz, Souillard, Lacroix [6] for $m > 1$. It is desirable to obtain similar equations for the evaluation of single or other combinations of the exponents.

In this paper the properties of a single transfer matrix are investigated. It will be proven that, for large n, half of its singular values have a lower bound that grows exponentially in n, and the other half have an upper bound that decays exponentially in n. Moreover, the spectrum of eigenvalues will be linked, via duality, to the spectrum of the difference equation (1) with proper boundary conditions.

The idea of duality is simple. For a chain of length n, if Bloch boundary conditions (b.c.) $u_{n+1} = e^{\mathrm{i}\varphi} u_1$ and $u_0 = e^{-\mathrm{i}\varphi} u_n$ are chosen (they correspond to an infinite periodic chain), an eigenvalue equation is obtained:

$$T(E) \begin{bmatrix} u_1 \\ u_0 \end{bmatrix} = e^{\mathrm{i}\varphi} \begin{bmatrix} u_1 \\ u_0 \end{bmatrix}. \tag{6}$$

The condition $\det[T(E) - e^{\mathrm{i}\varphi} \mathbb{I}_{2m}] = 0$ gives the nm eigenvalues $E_a(\varphi)$ of the difference equation (1). Then, for each eigenvalue, the whole eigenvector of the chain $(u_1 \ldots u_n)$ is constructed by applying the 1-step transfer matrices to the initial vector (u_1, u_0).

The opposite approach is also useful. The eigenvalue equation for $T(E)$

$$T(E) \begin{bmatrix} u_1 \\ u_0 \end{bmatrix} = z \begin{bmatrix} u_1 \\ u_0 \end{bmatrix} \tag{7}$$

is solved whenever $(u_1, \ldots, u_n)^t$ is an eigenvector with eigenvalue E of the matrix

$$H(z) = \begin{bmatrix} A_1 & B_1 & & \frac{1}{z} C_1 \\ C_2 & \ddots & \ddots & \\ & \ddots & \ddots & B_{n-1} \\ z B_n & & C_n & A_n \end{bmatrix} \tag{8}$$

which encodes the b.c. $u_{n+1} = z u_1$ and $u_0 = u_n / z$ that are implied by the eigenvalue equation for the transfer matrix. The statement

Proposition 1.1 *$(u_1, \ldots, u_n)^t$ is a right eigenvector with eigenvalue E of the matrix $H(z)$ if and only if $(u_1, u_n/z)^t$ is a right eigenvector of $T(E)$ with eigenvalue z,*

translates into a determinantal identity (the duality relation, [7]) that relates the eigenvalues of the tranfer matrix $T(E)$ to those the associated "Hamiltonian" matrix $H(z)$, that describes the difference equation of length n with generalized Bloch boundary conditions.

It is occasionally useful to replace the parameter z with z^n. The matrix $H(z^n)$ is similar to the balanced matrix

$$H^B(z) = \begin{bmatrix} A_1 & zB_1 & & \frac{1}{z}C_1 \\ \frac{1}{z}C_2 & \ddots & \ddots & \\ & \ddots & \ddots & zB_{n-1} \\ zB_n & & \frac{1}{z}C_n & A_n \end{bmatrix} \tag{9}$$

by the similarity relation $H(z^n) = D(z)H^B(z)D(z)^{-1}$, where $D(z)$ is the block diagonal matrix $(z\mathbb{I}_m, \ldots, z^n\mathbb{I}_m)$. As a consequence $H(z^n)$, $H^B(z)$ and also $H^B(ze^{\mathrm{i}k2\pi/n})$, $k = 1 \ldots n-1$, have the same eigenvalues.
While the matrix $H(z^n)$ remarks the value of z^n as a boundary condition parameter, the matrix $H^B(z)$ remarks the invariance under cyclic permutations of blocks (the ring geometry) of the difference equation (and is numerically more tractable).

Tridiagonal matrices of type (9), with $z = e^\xi$ real, were introduced by Hatano and Nelson [8] to model vortex pinning in superconductors:

$$e^\xi u_{k+1} + a_k u_k + e^{-\xi} u_{k-1} = E u_k,$$

where a_k are independent random entries. The model attracted a great interest as it gave another view of the relationship between localization and spectral response to b.c. variations. For zero or small ξ the eigenvalues are real and all eigenvectors are exponentially localized with localization lengths $1/\lambda(E)$. The Lyapunov exponent can be evaluated by Thouless' formula (5), $\lambda(E) = \int dE\rho(E) \ln|E - E'|$, with the average spectral density of the Hermitian chain (the analytic evaluation is possible in Lloyd's model, with Cauchy disorder [9]). By increasing ξ beyond a critical value the eigenvalues start to gain imaginary parts and distribute along a single expanding curve [10] of equation $\xi = \lambda(E)$ (see figure 1). The transition has been studied also in 2D, where the critical value of ξ for the onset of migration in the complex plane gives the inverse localization in the center of the band [11].
If the parameter ξ is turned on in tridiagonal random matrices that are not Hermitian at the beginning,

$$b_k e^\xi u_{k+1} + a_k u_k + e^{-\xi} c_k u_{k-1} = E u_k,$$

the phenomenon shows up differently [12]: beyond a critical value of ξ, an area occupied by the complex eigenvalues starts to be depleted, the eigenvalues being swept away and accumulated on an expanding "front line" of equation $\xi = \lambda(E)$. No eigenvalues are left in the interior (corresponding to delocalization of states) (see figure 2).

Though the theory presented in this paper is very general, these two models were the starting motivation:
1) **band random matrices** have block tridiagonal structure with lower and upper triangular B and C matrices. Matrix elements are independent and identically distributed (i.i.d.) random variables. It is customary to name m as b (bandwidth

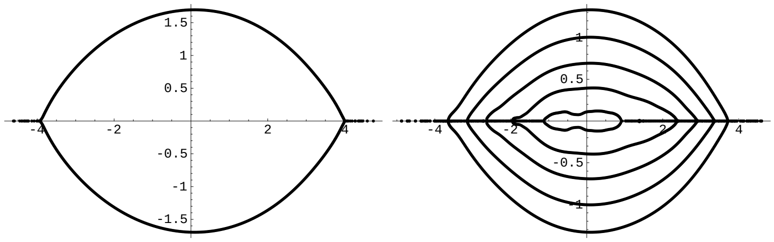

Figure 1. Left: the complex eigenvalues of a Hatano Nelson tridiagonal matrix ($m = 1$, $n = 600$, $\xi = 1$) with random diagonal elements uniformly chosen in $[-3.5, +3.5]$. They lie on the line $\xi = \lambda(E)$. The real eigenvalues correspond to states with localization length less than $1/\xi$. Right: the same system, with ξ increasing from 0 to 1 in five steps to show the expanding spectral curve.

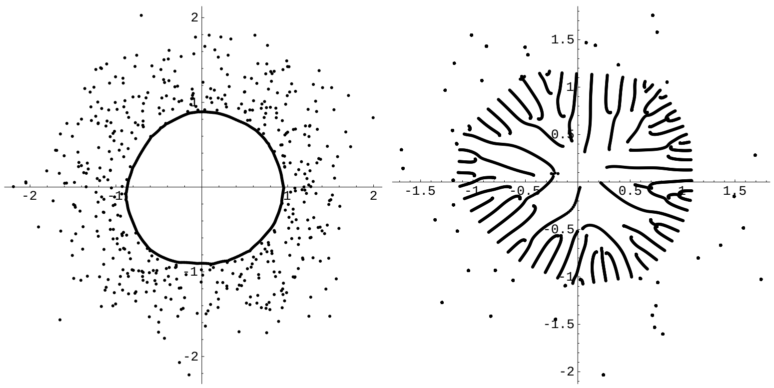

Figure 2. Left: the eigenvalues of a tridiagonal matrix ($m = 1$, $n = 800$, $\xi = 0.5$) with elements a_k, b_k, c_k chosen uniformly in $[-1, 1]$; the "front circle" contains the eigenvalues that filled the circle at lower values of ξ. Right: the motion of eigenvalues ($n = 100$) is traced for ξ changing from 0.3 to 0.6. The outer eigenvalues are numerically unaffected before being reached by the "front circle".

is $2b + 1$). If the probability distribution has zero mean and finite variance, and if $n \gg b \gg 1$, the spectral density of Hermitian banded matrices is Wigner's semicircle law, with exponentially localized eigenvectors. The localization length and its finite size scaling were studied numerically by Casati et al.[13], with insight provided by the kicked rotor model of quantum chaos. Several properties were obtained analytically by supersymmetric techniques in a series of papers by Fyodorov and Mirlin [14].

2) **Anderson model** describes the propagation of a particle in a lattice with random site potential. After choosing a (long) direction of length n, the diagonal blocks $A_k = T + D_k$ describe the sections of the lattice with m sites each (T is the Laplacian matrix for the transverse slice and D_k is a random diagonal matrix with i.i.d. elements). The hopping among neighboring slices is fixed by $B_k = C_k = \mathbb{I}_m$. The random site-potential is usually chosen uniformly distributed in $[-w/2, w/2]$ (w is the disorder parameter) (the literature is vast, see [15] for a mathematical introduction).

In both models the transfer matrix is a product of random matrices and, for $n \to \infty$,

it provides a non random Lyapunov spectrum [16, 17, 18]. The inverse of the smallest Lyapunov exponent is the localization length.
Localization affects the response of energy values to variations of b.c. [19, 20]. This dual way of viewing localization: through decay of eigenvectors (transfer matrix) or response of energy levels to b.c. variations (Hamiltonian matrix), is hidden in the duality identity among the eigenvalues of $T(E)$ and of $H(z)$.

Finally, let's briefly mention the scattering approach to transport and localization, introduced by R. Landauer in 1957. The finite chain is coupled to two infinite ordered chains (the leads) which sustain Bloch waves that are transmitted and reflected by the chain. The transmission matrix is evaluated through the transfer matrix (or the related scattering matrix) of the finite chain. Its singular values give the conductance properties of the chain. The literature is vast and is also accessible in books [21].

The first two sections provide algebraic properties that relate a generic transfer matrix to its Hamiltonian matrix. Some of them appeared in previous papers, but receive here a consistent presentation. In particular, they are the spectral duality and the expression of $T(E)$ in terms of the resolvent of the Hamiltonian matrix with open b.c.
Next, a theorem by Demko, Moss and Smith [22] on the decay of matrix elements of the inverse of a banded matrix is presented. It is used here to prove that a $2m\times 2m$ transfer matrix has m singular values growing exponentially with the length of the chain, and m singular values decaying exponentially. This new result reflects on a single matrix a property of random matrix products.
The rest of the paper deals with identities; duality and Jensen's identity give an expression for the exponents $\xi_a = \frac{1}{n}\ln|z_a|$, where z_a are the eigenvalues of the transfer matrix, in terms of the eigenvalues of the associated matrix $H(z)$. Hadamard's inequality for determinants of positive matrices supports the idea that the eigenvalues z_a have a leading exponential growth in n. The discussion of the relevant case of Hermitian difference equation ends the paper.

2. Transfer matrix and duality

Some general facts about transfer matrices are presented. By construction $T(E)$ is a polynomial in E of degree n, $T(E) = E^n T_n + \ldots + ET_1 + T_0$, with matrix coefficients. However, its determinant is independent of E:

$$\det T(E) = \prod_{k=1}^{n} \det t_k(E) = \frac{\det[C_1 \cdots C_n]}{\det[B_1 \cdots B_n]} \tag{10}$$

This implies that $T(E)^{-1}$ is again a matrix polynomial in E [23]. Actually $T(E)^{-1}$ is similar to the transfer matrix of the inverted chain. Let's introduce the two matrices of inversion, of size $2m \times 2m$ and $nm \times nm$:

$$\sigma_x =: \begin{bmatrix} 0 & \mathbb{I}_m \\ \mathbb{I}_m & 0 \end{bmatrix}, \qquad J = \begin{bmatrix} & & \mathbb{I}_m \\ & \cdots & \\ \mathbb{I}_m & & \end{bmatrix},$$

Proposition 2.1 *Let $T(E)$ be a transfer matrix and $H(z)$ the associated matrix, and let $T(E)^J$ be the transfer matrix associated to $H^J(z) = JH(z)J$ (the inverted chain); then: $T(E)^{-1} = \sigma_x T(E)^J \sigma_x$.*
Proof: $T(E)^{-1} = [t_n(E)\cdots t_1(E)]^{-1} = t_1(E)^{-1}\cdots t_n(E)^{-1}$. The combination

$$\sigma_x\, t_k^{-1}\sigma_x = \begin{bmatrix} C_k^{-1}(E-A_k) & -C_k^{-1}B_k \\ \mathbb{I}_m & 0 \end{bmatrix}$$

gives the structure of a 1-step transfer matrix. Multiplication yields the result. □

Proposition 2.2 *In the expansion of the characteristic polynomial of the transfer matrix,*

$$\det\,[z\mathbb{I}_{2m} - T(E)] = \, z^{2m} + \ldots + a_k(E)z^{2m-k} + \ldots + a_{2m-k}(E)z^k + \ldots + a_{2m},$$

the coefficients $a_k(E)$ and $a_{2m-k}(E)$ are (in general different) polynomials in E of degree kn $(k = 0, ..., m)$.
Proof: Let $z_1, \ldots, z_{2m}$ be the eigenvalues of $T(E)$. The coefficients

$$a_k = (-1)^k \sum_{i_1<\ldots<i_k} z_{i_1}\cdots z_{i_k}, \qquad k = 1\ldots m,$$

can be expressed as combination of traces of powers of $T(E)$ of degree k: $a_1 = -\,\mathrm{tr}\; T(E)$, $a_2 = \frac{1}{2}[\mathrm{tr}\; T(E)]^2 - \frac{1}{2}\,\mathrm{tr}\,[T(E)^2]$, etc. Since $T(E) = E^nT_n + \ldots + T_0$, the coefficient a_k is a polynomial of degree kn in E. The remaining coefficients a_{2m-k} are discussed differently. The point is that $a_{2m} = z_1\cdots z_{2m} = \det T(E)$ is independent of E and the coefficients can be written as

$$a_{2m-k} = (-1)^k \sum_{i_1<\ldots<i_{2m-k}} z_{i_1}\cdots z_{i_{2m-k}} = (-1)^k a_{2m} \sum_{i_1<\ldots<i_k} (z_{i_1}\cdots z_{i_k})^{-1}$$

Therefore, $a_{2m-1} = -a_{2m}\;\mathrm{tr}[T(E)^{-1}]$, $a_{2m-2} = a_{2m}\frac{1}{2}[\mathrm{tr}\,T(E)^{-1}]^2 - a_{2m}\frac{1}{2}\,\mathrm{tr}[T(E)^{-2}]$, etc. Since also $T(E)^{-1}$ is a polynomial matrix of degree n in E, a_{2m-k} is a polynomial of degree kn in E. □

Theorem 2.3 (Duality)

$$\det[z\mathbb{I}_{2m} - T(E)] = (-z)^m \frac{\det[E\mathbb{I}_{nm} - H(z)]}{\det(B_1\cdots B_n)} \tag{11}$$

Proof: According to proposition 2.2 the leading term in the expansion in E of $\det\,[z\mathbb{I}_{2m} - T(E)]$ coincides with the leading term in the expansion of $\det[z\mathbb{I}_{2m} - E^nT_n]$, which is $(-z)^m E^{nm}\det[B_1\cdots B_n]^{-1}$. The leading term of $\det[E\mathbb{I}_{2m} - H(z)]$ is E^{nm}. Since by proposition 1.1 the two polynomials, for given z, have the same zeros in E, they must be proportional by a constant. □

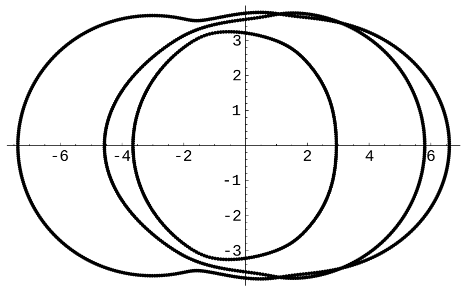

Figure 3. The eigenvalues of the Hamiltonian matrix ($n = 8, m = 3$) of a 2D Anderson model on a lattice 3×8, diagonal disorder parameter $w = 7$. The b.c. parameter is $z = \exp(n\xi + i\varphi)$ with $\xi = 1.5$. As φ changes, the 24 eigenvalues (of the balanced matrix) trace $m = 3$ closed loops of equation $\ln|z_k(E)| = 1.5$.

This relation among characteristic polynomials is a "duality identity" as it exchanges the roles of the parameters z and E among the two matrices: z is an eigenvalue of $T(E)$ if and only if E is an eigenvalue of the block tridiagonal matrix $H(z)$. I gave different proofs of it [7, 24, 25]. With $z = 1$ it is a tool for computing determinants of block tridiagonal or banded matrices with corners.
The eigenvalues of $H(z)$ make the l.h.s. of duality equal to zero, i.e. there is at least a complex factor $z_i(E) - z = 0$. This means that an eigenvalue E is at the intersection of a line $|z_i(E)| = |z|$ and arg $z_i(E) =$arg z. By changing only the parameter arg z, the eigenvalues move along *spectral lines* $|z_i(E)| = |z|$. For tridiagonal matrices ($m = 1$) there is a single spectral curve (figure 1), for $m > 1$ several spectral curves appear [26] (see figure 3).

A more symmetric duality relation results from multiplication of the dual identities for $(T - z)$ and $(T - 1/z)$:

$$\det\left[T(E) + T(E)^{-1} - \left(z + \frac{1}{z}\right)\mathbb{I}_{2m}\right] = \frac{\det[E\mathbb{I}_{nm} - H(z)]\,\det[E\mathbb{I}_{nm} - H(1/z)]}{\det[B_1\cdots B_n]\,\det[C_1\cdots C_n]}$$

3. Transfer matrix and resolvent

Equation (1) with open b.c. $u_0 = 0$ and $u_{n+1} = 0$, is the eigenvalue equation for the matrix

$$h = \begin{bmatrix} A_1 & B_1 & & \\ C_2 & \ddots & \ddots & \\ & \ddots & \ddots & B_{n-1} \\ & & C_n & A_n \end{bmatrix} \tag{12}$$

Let $(u_1, \ldots, u_n)^t$ be a (right) eigenvector of h with eigenvalue E; then u_1 and u_n are both nonzero, or the whole vector would be null by the chain recursion. With the block partition

$$T(E) = \begin{bmatrix} T(E)_{1,1} & T(E)_{1,2} \\ T(E)_{2,1} & T(E)_{2,2} \end{bmatrix}$$

(3) gives $T(E)_{1,1}u_1 = 0$ and $T(E)_{2,1}u_1 = u_n$. This means that $\det T(E)_{1,1} = 0$ whenever $\det[E\mathbb{I}_{nm} - h] = 0$ (and $\det T(E)_{2,1} \neq 0$). The following duality relation results:

Proposition 3.1 (duality for the open chain)

$$\det[E\mathbb{I}_{nm} - h] \;=\; \det T(E)_{1,1}\, \det[B_1 \cdots B_n] \tag{13}$$

Proof: by construction $T(E)_{11} = E^n (B_1 \cdots B_n)^{-1} +$ lower powers in E. Then both $\det[E\mathbb{I}_{nm} - h]$ and $\det T(E)_{11}$ are polynomials in E of degree nm. Having the same roots, they are proportional. □

The blocks $T(E)_{12}$ and $T(E)_{21}$ are polynomial matrices of degree $n-1$ in E, and $T(E)_{22}$ has degree $n-2$. The four blocks can be evaluated in terms of the corner blocks of the resolvent matrix

$$g(E) = [h - E\mathbb{I}_{nm}]^{-1} =: \begin{bmatrix} g_{1,1} & \cdots & g_{1,n} \\ \vdots & & \vdots \\ g_{n,1} & \cdots & g_{n,n} \end{bmatrix}$$

The corner matrices C_1 and B_n are absent in h but enter in the definition of $T(E)$ through the 1-step factors $t_1(E)$ and $t_n(E)$, and will be accounted for.

Proposition 3.2 *Let $g_{i,j} \in \mathbb{C}^{m\times m}$ $(a, b = 1 \dots n)$ be the blocks of $g(E)$. Then*

$$T(E) = \begin{bmatrix} -B_n^{-1}(g_{1,n})^{-1} & -B_n^{-1}(g_{1,n})^{-1} g_{1,1} C_1 \\ g_{n,n}(g_{1,n})^{-1} & g_{n,n}(g_{1,n})^{-1} g_{1,1} C_1 - g_{n,1} C_1 \end{bmatrix} \tag{14}$$

Proof: write the identity $[h - E\mathbb{I}_{nm}]g(E) = \mathbb{I}_{nm}$ for the block indices $i = 2 \dots n-1$ and $k = 1, n$: $C_i g_{i-1,k} + (A_i - E\mathbb{I}_m) g_{ik} + B_i g_{i+1,k} = 0$. The recursive relations are solved by the transfer matrix method and give a matrix relation among the corner blocks:

$$\begin{bmatrix} g_{n,1} & g_{n,n} \\ g_{n-1,1} & g_{n-1,n} \end{bmatrix} = t_{n-1}(E) \cdots t_2(E) \begin{bmatrix} g_{2,1} & g_{2,n} \\ g_{1,1} & g_{1,n} \end{bmatrix}$$

Left multiply both sides by $t_n(E)$ and simplify l.h.s. by means of the identity $C_n g_{n-1,k} + (A_n - E\mathbb{I}_m) g_{n,k} = \delta_{k,n}\mathbb{I}_m$. Insert $t_1(E)t_1(E)^{-1} = \mathbb{I}_{2m}$ in the r.h.s. to obtain $T(E)t_1^{-1}$, and simplify the action of t_1^{-1} by means of the identity $(A_1 - E\mathbb{I}_m) g_{1,k} + B_1 g_{2,k} = \delta_{1,k}\mathbb{I}_m$. The useful factorization is obtained:

$$\begin{bmatrix} 0 & -B_n^{-1} \\ g_{n,1} & g_{n,n} \end{bmatrix} = T(E) \begin{bmatrix} g_{1,1} & g_{1,n} \\ -C_1^{-1} & 0 \end{bmatrix} \tag{15}$$

A matrix inversion and multiplication give the result. □

Remark 3.3 *The representation provides the transfer matrix through a large matrix inversion, rather than multiplications. The blocks T_{ij}, corrected by the velocities of the channels of the leads [7], provide the transmission and the reflection matrices. The relation between the transmission matrix and the resolvent was first obtained by D. Fisher and P. Lee [27]. It was used by Kramer and MacKinnon [28] in a numerical proof of one-parameter scaling for the localization length of Anderson's model.*

4. Exponential inequalities

Products of random matrices are known to exhibit Lyapunov exponents that are asymptotically stable and self-averaging, i.e. independent of the length n and of the realization of the random product. In the present deterministic approach a single chain is considered, and it will be shown that it is possible to give exponential bounds on the eigenvalues for long chains, that justify the introduction of exponents.

Demko, Moss and Smith [22] made the very general statement that, loosely speaking, the matrix elements of the inverse of block tridiagonal or banded matrices *decay exponentially from the diagonal* (see also [29, 30]). I here present their interesting proof adapted to the block partitioning of matrices. I then apply it to the matrix $g(E)$ to obtain bounds for the singular values of $T(E)$.

The main ingredient is the best approximation of the function $(x-a)^{-1}$ on the interval $[-1,1]$ ($|a|>1$) by a polynomial of degree k, which was obtained by Chebyshev together with the determination of the error [31]. With proper rescaling it is [22]:

Lemma 4.1 *Let P_k be the set of real monic polynomials of degree k, let $[a,b]$ be an interval of the positive real line, with $a>0$. Then:*

$$\inf_{p\in P_k}\left\{\sup_{x\in[a,b]}\left|\frac{1}{x}-p(x)\right|\right\} = C\, q^{k+1}, \tag{16}$$

$$C=\frac{(\sqrt{b}+\sqrt{a})^2}{2ab}, \qquad q=\frac{\sqrt{b}-\sqrt{a}}{\sqrt{b}+\sqrt{a}} \tag{17}$$

If A is a block tridiagonal matrix with blocks of size $m\times m$ and if $p_k(x)$ is a polynomial of degree k, the blocks $p_k(A)_{i,j}$ of the matrix $p_k(A)$ are null for $|i-j|>k$.
Let A be a positive definite block tridiagonal matrix, with inverse A^{-1}. If $A^{-1}[i,j]$ denotes any matrix element in the block $(A^{-1})_{ij}$ then, for any monic real polynomial of degree $k=|i-j|-1$, it is:

$$\begin{aligned}|A^{-1}[i,j]| &= \left|A^{-1}[i,j]-p_k(A)[i,j]\right| \\ &\le \|A^{-1}-p_k(A)\| = \sup_{\lambda\in sp(A)}\left|\frac{1}{\lambda}-p_k(\lambda)\right| \\ &\le \sup_{\lambda\in[a,b]}\left|\frac{1}{\lambda}-p_k(\lambda)\right|\end{aligned}$$

where $\|A\|=\sup_{\|x\|=1}\|Ax\|$ is the operator norm‡, and the spectral theorem is used. In the last line $[a,b]$ is the smallest interval containing the spectrum of eigenvalues $sp(A)$. Next, the inf is taken over the polynomials p_k. The lemma states that the minimum exists, and the error gives the main inequality. Note that for $|i-j|=0$: $|A^{-1}[i,i]|\le\|A^{-1}\|=1/a$. Therefore:

‡ For any matrix A with matrix elements A_{rs} it is $|A_{rs}|=|(e_r|Ae_s)|\le\|Ae_s\|\le\|A\|$, where e_i are canonical unit vectors and Schwarz's inequality is used.

Theorem 4.2 (Demko, Moss and Smith) *Let A be a positive definite block tridiagonal matrix, with square blocks of size m, let $[a,b]$ be the smallest interval containing the spectrum of A, let $A^{-1}[i,j]$ be any matrix element in the block $(A^{-1})_{ij}$. Then:*

$$\left|A^{-1}[i,j]\right| \le \begin{cases} C\, q^{|i-j|} & \text{for } |i-j|\ge 1 \\ 1/a & \text{for } i=j \end{cases} \tag{18}$$

where $q<1$ and C are specified by eq.(17).

Demko et al. also proved an extension of the theorem to a matrix A that is block tridiagonal invertible but fails to be positive. An estimate for A^{-1} is obtained by noting that $A^{-1} = A^\dagger (AA^\dagger)^{-1}$. The matrix $AA^\dagger$ is block 5-diagonal positive definite, and a polynomial $p_k(AA^\dagger)$ is a matrix whose blocks (i,j) are null if $|i-j|>2k$. The previous theorem applies, with $[a,b]$ being the smallest positive interval containing $sp(AA^\dagger)$:

$$|(AA^\dagger)^{-1}[i,j]| \le \frac{C}{\sqrt{q}}\, q^{\frac{1}{2}|i-j|}, \quad |i-j|>2$$

The extension of the theorem is here written in the block notation, with minor changes from the original paper:

Theorem 4.3 *Let A be an invertible block tridiagonal matrix with square blocks of size m, let $[a,b]$ be the smallest interval containing $sp(A^\dagger A)$, let $A^{-1}[i,j]$ be any matrix element in the block $(A^{-1})_{ij}$. Then:*

$$|A^{-1}[i,j]| \le C_i\, q^{\frac{1}{2}|i-j|} \tag{19}$$

$$C_i = \frac{C}{q}\left(\|A_{i-1,i}\| + \|A_{i,i}\| + \|A_{i+1,1}\|\right), \tag{20}$$

where $q<1$ and C are given in (17).

Proof: in terms of block multiplication:

$$(A^{-1})_{ij} = (A^\dagger)_{i,i-1}[(AA^\dagger)^{-1}]_{i-1,j} + (A^\dagger)_{i,i}[(AA^\dagger)^{-1}]_{i,j} + (A^\dagger)_{i,i+1}[(AA^\dagger)^{-1}]_{i+1,j}.$$

The sup norm, the triangle inequality, the property $\|AB\|\le\|A\|\|B\|$, and the bound on $(AA^\dagger)^{-1}$ give:

$$\begin{aligned}\|(A^{-1})_{ij}\| &\le \|A_{i-1,i}\|\|(AA^\dagger)^{-1}{}_{i-1,j}\| + \|A_{i,i}\|\|(AA^\dagger)^{-1}{}_{i,j}\| + \|A_{i+1,i}\|\|(AA^\dagger)^{-1}{}_{i+1,j}\| \\ &\le \frac{C}{\sqrt{q}}\left(\|A_{i-1,i}\|q^{\frac{1}{2}|i-j-1|} + \|A_{i,i}\|q^{\frac{1}{2}|i-j|} + \|A_{i+1,i}\|q^{\frac{1}{2}|i-j+1|}\right) \\ &\le \frac{C}{q}\left(\|A_{i-1,i}\| + \|A_{i,i}\| + \|A_{i+1,j}\|\right)\; q^{\frac{1}{2}|i-j|}\end{aligned}$$

If $A^{-1}[i,j]$ is any matrix element in the block $(A^{-1})_{ij}$, it is $|A^{-1}[i,j]| \le \|(A^{-1})_{ij}\|$. $\square$

Given an invertible matrix A, the *condition number* of A is [2]:

$$\text{cond (A)} =: \|\text{A}\|\,\|\text{A}^{-1}\|$$

In general it is cond $(A)\ge 1$. If a and b are the extrema of the spectrum of a positive matrix P it is $b=\|P\|$ and $1/a = \|P^{-1}\|$; then $b/a = $ cond (P).

Since $\|AA^\dagger\| = \|A\|^2$, it is cond $(AA^\dagger) = [\mathrm{cond(A)}]^2$ and the parameters in theorem 4.3 are:

$$q = \frac{\mathrm{cond(A)} - 1}{\mathrm{cond(A)} + 1}, \qquad C = \frac{(\mathrm{cond(A)} + 1)^2}{2\|A\|^2} \tag{21}$$

Theorem 4.3 is applied to the corner blocks of the resolvent $g(E) = [h - E\mathbb{I}_{nm}]^{-1}$, $E \notin sp(h)$, which enter in the representation (14) of the transfer matrix. The numbers cond $(h - E)$ and $\|h - E\|$ define the parameters $q < 1$ and C.

Proposition 4.4 *If $g[1,n]$ and $g[n,1]$ are matrix elements of the corner blocks g_{1n} and g_{n1} of $g(E)$, then the following inequalities hold:*

$$|g[1,n]| \;\le\; C\,(\|A_1 - E\| + \|B_1\|)q^{\frac{1}{2}(n-3)}, \tag{22}$$
$$|g[n,1]| \;\le\; C\,(\|A_n - E\| + \|C_n\|)q^{\frac{1}{2}(n-3)} \tag{23}$$

where A_1, B_1, A_n, B_n are the blocks in the first and last row of h.

We prepare for the main theorem with the following lemma:

Lemma 4.5 *The singular values θ_k of the block T_{11} of $T(E)$ are exponentially large in n: $\theta_k > q^{-n/2}/K$.*
Proof: from $(T_{11})^{-1} = -g_{1n}B_n$ it follows that: $\mathrm{tr}[(T_{11}^\dagger T_{11})^{-1}] = \mathrm{tr}[B_nB_n^\dagger g_{1n}^\dagger g_{1n}] \le m^2\|B_nB_n^\dagger\|\|g_{1n}^\dagger g_{1n}\| = m^2\|B_n\|^2\|g_{1n}\|^2 \le m^2\|B_n\|^2C^2(\|A_1 - E)\| + \|B_1\|)^2q^{n-3} =: K^2\,q^n$. Since $\mathrm{tr}[(T_{11}^\dagger T_{11})^{-1}] = \sum_{k=1}^m \theta_k^{-2}$, it turns out that each singular value of T_{11} is larger than $q^{-n/2}/K$. □

Main Theorem 4.1 *If $q < 1$ and n is large, the transfer matrix $T(E)$ has m singular values larger than $\frac{1}{K}q^{-n/2}$ and m singular values smaller than $Kq^{n/2}$.*
Proof: Let $\theta_1 \ge \ldots \ge \theta_m$ be the singular values of the block T_{11}, and let $\sigma_1 \ge \ldots \ge \sigma_{2m}$ be the singular values of $T(E)$. The interlacing property (Theorem 7.12 of ref.[32]) states that:

$$\sigma_k \ge \theta_k \ge \sigma_{m+k}, \quad k = 1, \ldots, m$$

Therefore, there are at least m singular values of $T(E)$ that are larger than $\frac{1}{K}q^{-n/2}$. Since the same conclusion holds true for $T(E)^{-1}$, which is similar to a transfer matrix by proposition 2.1, there are precisely m singular values of $T(E)$ that are larger than $\frac{1}{K}q^{-n/2}$, and m that are smaller than $Kq^{n/2}$. □

5. Jensen's formula and the exponents

The two sides of the duality relation are determinantal expressions of the same polynomial in two variables, $F(z,E) =: \det\,[z\mathbb{I}_{2m} - T(E)]$. Let $z_1, \ldots, z_{2m}$ be the zeros in the variable z (the eigenvalues of $T(E)$) with $|z_1| \ge \ldots \ge |z_{2m}|$, and let $E_1, \ldots, E_{nm}$ be the zeros in E (the eigenvalues of $H(z)$). It is convenient to introduce the *exponents* of the transfer matrix:

$$\xi_k =: \frac{1}{n}\ln|z_k|$$

Remark 5.1 *The exponents are not to be confused with the Lyapunov exponents, which are defined in terms of the positive eigenvalues σ_k^2 of the matrix $T^\dagger T$. It has been shown (with less general T) that also $T^\dagger T$ is the transfer matrix of a block tridiagonal matrix, so the same discussion may be applied to them [26].*

The sum of the exponents is $\frac{1}{n}\ln|\det T(E)|$. Then:

$$\sum_{k=1}^{2m}\xi_k = \frac{1}{n}\sum_{j=1}^{n}(\ln|\det C_j| - \ln|\det B_j|) \tag{24}$$

Some general analytic results are now given, based on the following theorem of complex anaysis [33]:

Theorem 5.2 (Jensen) *If f is holomorphic and $f(0)\neq 0$, and $z_1\dots z_n$ are its zeros in the disk of radius r, then: $\int_0^{2\pi}\frac{d\theta}{2\pi}\ln|f(re^{\mathrm{i}\theta})| = \ln|f(0)| - \sum_k \ln(|z_k|/r)$.*

The theorem is applied to $F(z,E)$ as a function of z, resulting in a relation between a sum of the exponents and the spectrum of the Hamiltonian matrix [34]:

Proposition 5.3

$$\frac{1}{m}\sum_{\xi_k<\xi}(\xi-\xi_k) \; -\xi$$

$$= \frac{1}{mn}\int_0^{2\pi}\frac{d\varphi}{2\pi}\ln|\det[H(\exp[n\xi+\mathrm{i}\varphi]) - E]| - \frac{1}{mn}\sum_{j=1}^{n}\ln|\det\, C_j| \tag{25}$$

Proof: Jensen's theorem with $z = e^{n\xi+\mathrm{i}\theta}$ gives in the r.h.s. the sum of exponents contained in the disk of radius $e^{n\xi}$:

$$\int_0^{2\pi}\frac{d\theta}{2\pi}\ln\left|F(e^{n\xi+\mathrm{i}\theta},E)\right| = \ln|\det T(E)| + n\sum_{k=1}^{2m}(\xi-\xi_k)\theta(\xi-\xi_k).$$

The dual expression is used in the l.h.s.: $\ln|F| = mn\xi + \ln|\det[H(e^{n\xi+\mathrm{i}\varphi}) - E]| - \sum_j \ln|\det B_j|$. □

A derivative in the variable ξ of (25) gives the counting functions of exponents $N(\xi,E) = \sum\theta(\xi-\xi_a(E))$, which is also obtainable by Euler's formula for the zeros z_k of the entire function $F(z,E)$ [37].

Hadamard-Fisher's inequality [2, 32] states that if $M_1,\dots,M_n$ are the diagonal blocks of the positive matrix $A^\dagger A$, then $|\det A|^2 \le \det M_1\cdots\det M_n$.
The inequality is applied to the r.h.s. in eq.(25), with the balanced matrix $H^B(e^{\xi+\mathrm{i}\varphi/n})$:

$$\sum_{k=1}^{2m}(\xi-\xi_k)\theta(\xi-\xi_k) - m\xi \le -\frac{1}{n}\sum_{j=1}^{n}\ln|\det\, C_j| \tag{26}$$

$$+\frac{1}{2n}\sum_{k=1}^{n}\ln\det\left[(A_k^\dagger - \overline{E})(A_k - E) + e^{2\xi}B_k^\dagger B_k + e^{-2\xi}C_k^\dagger C_k\right]$$

If the norms of matrices A_i B_i and C_i are bounded by some constant for all i, and m is fixed, the sum in l.h.s. of inequality remains finite for any length n, as the r.h.s. is an average value for the blocks.

Corollary 5.4 *The sum of the positive exponents is obtained from (25) with $\xi = 0$ and by means of eq.(24)*

$$\sum_{k=1}^{2m} \xi_k\, \theta(\xi_k) = \frac{1}{n}\int_0^{2\pi} \frac{d\theta}{2\pi} \ln\left|\det[H(e^{i\theta}) - E]\right| - \frac{1}{n}\ln|\det[B_1 \cdots B_n]| \tag{27}$$

The identity is exact and applies to a single transfer matrix. It is reminiscent of the formula (5) for the sum of the Lyapunov exponents of random transfer matrices. The "angular average" replaces the ensemble averaged density of eigenvalues $\rho(E)$, which was extended to tridiagonal non-Hermitian matrices in [35, 36].

6. The Hermitian difference equation

Most of the literature concentrates on the Hermitian case. However, as duality requires z to be a complex parameter, the matrix $H(z)$ fails to be Hermitian unless $|z| = 1$;

$$H(z) = \begin{bmatrix} A_1 & B_1 & & \frac{1}{z}B_n^\dagger \\ B_1^\dagger & \ddots & \ddots & \\ & \ddots & \ddots & B_{n-1} \\ zB_n & & B_{n-1}^\dagger & A_n \end{bmatrix}, \qquad A_k = A_k^\dagger \tag{28}$$

A useful symplectic property holds for the transfer matrix (in transport problems it describes flux conservation, [7]), and implies that exponents come in pairs $\pm\xi_a$:

Proposition 6.1 $$T(\overline{E})^\dagger \Sigma_n T(E) = \Sigma_n, \qquad \Sigma_n = i\begin{bmatrix} 0 & -B_n^\dagger \\ B_n & 0 \end{bmatrix} \tag{29}$$

Proof: in the factorization $T(E) = t_n(E)\cdots t_1(E)$, the factors $t_k(E)$ $(k = 2 \dots n)$ have the property $t_k(\overline{E})^\dagger \Sigma_k t_k(E) = \Sigma_{k-1}$. The factor t_1 that contains the boundary blocks, closes the loop: $t_1(\overline{E})^\dagger \Sigma_1 t_1(E) = \Sigma_n$. □

Corollary 6.2 *If E is real, the eigenvalues of $T(E)$ different from ± 1 come in pairs z, $1/\overline{z}$. The associated exponents are opposite.*
Proof: If $T(E)u = zu$, the symplectic property implies that $T(E)^\dagger \Sigma_n u = 1/z \Sigma_n u$ i.e. $1/\overline{z}$ is an eigenvalue of $T(E)$. Moreover, if $|z| \neq 1$, then $u^\dagger \Sigma_n u = 0$.

Proposition 6.3 *If Im $E \neq 0$ then $T(E)$ has no eigenvalues on the unit circle.*
Proof: for Im $E \neq 0$ and $z = e^{i\theta}$ it is always $\det[E - H(e^{i\theta})] \neq 0$ because $H(e^{i\theta})$ is Hermitian and it has real eigenvalues. Therefore, by duality, $\det[T(E) - e^{i\theta}\mathbb{I}_{2m}]$ never vanishes. □

A degeneracy occurs in the exponents of the real transfer matrix of a real symmetric difference equation (the Anderson model is a notable example, but remind remark 5.1):

Proposition 6.4 *Let the matrices A_k be real symmetric and B_k be real invertible. For $E \in \mathbb{R}$, the real eigenvalues of $T(E)$ come in pairs z, $1/z$, the complex ones also have the conjugated pair $\overline{z}$, $1/\overline{z}$.*

Proof: if z is a complex eigenvalue of $T(E)$ not in the unit circle, then also $\overline{z}$, $1/\overline{z}$ and $1/z$ are distinct eigenvalues, and exponents are doubly degenerate opposite pairs. If z is a real eigenvalue, then $1/z$ is an eigenvalue. Therefore an eigenvalue (real or not) is always paired to the eigenvalue $1/z$. $\square$

Conclusions

Even for general transfer matrices of block tridiagonal matrices one can make several analytic statements. For any number n of matrix factors, the eigenvalues of the transfer matrix are related to those of the block tridiagonal matrix by duality and Thouless-like identities, with a parameter that allows to scan the spectrum. It would be a great achievement to implement such exact formulae in the study of the Lyapunov spectrum of the Anderson model.
Next, it is here shown that, for large n, the singular values of the transfer matrix either decay or grow (in equal number) with increasing n. This reflects the large n behaviour of the matrix elements of the inverse of any band matrix, described in the theorem by Demko, Moss and Smith.

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