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Transfer matrices and tridiagonal-block Hamiltonians with periodic and scattering boundary conditions

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Abstract. General Hamiltonian matrices with tridiagonal block structure and the associated transfer matrices are investigated in the cases of periodic and scattering boundary conditions. They arise from tight binding models with finite range hopping in one or more dimensions of space, in the presence of a Aharonov–Bohm flux or in multichannel scattering. An identity relating the characteristic equation of the periodic Hamiltonian with that of the transfer matrix is found, allowing a detailed analysis of the bands. A velocity matrix is defined, with properties relevant for the band structure, or for the channel structure in the scattering problem.

1. Introduction

Several interesting physical systems are described by Hamiltonians which are directly formulated as Jacobi matrices. A significative and very investigated class is given by lattice models for one-dimensional transport with disorder [1–9]. In the simplest version, the Hamiltonian is the sum of a kinetic term with equal amplitudes for hopping to nearest-neighbouring sites, and a site-potential term which describes the disorder

$$(H\psi)_n = -\psi_{n+1} - \psi_{n-1} + \epsilon_n \psi_n. \tag{1.1}$$

The tridiagonal structure is particularly suitable both for the numerical and the theoretical analysis, the latter being usually based on the powerful concept of transfer matrix. In the example, given the solution of the eigenvalue equation $(H\psi)_n = E\psi_n$ with certain boundary conditions, the transfer matrix connects components at different sites via a multiplicative process with basic step

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = T_n(E) \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} \qquad T_n(E) = \begin{pmatrix} \epsilon_n - E & -1 \\ 1 & 0 \end{pmatrix}. \tag{1.2}$$

The eigenvalues z, $1/z$ of the transfer matrix $T(E) = T_N(E) \dots T_1(E)$ for a chain of length N are related to those of the Hamiltonian matrix $H_N(p)$ with periodic boundary conditions $\psi_{N+1} = \mathrm{e}^{\mathrm{i}p}\psi_1$, $\psi_0 = \mathrm{e}^{-\mathrm{i}p}\psi_N$, as it occurs for a ring with a magnetic flux through it, through the equality [7, 10]

$$\det[E - H_N(p)] = z + \frac{1}{z} - 2\cos p. \tag{1.3}$$

The first and second derivatives of the energy values $E_i(p)$ are known as level velocity and curvature, and describe the sensitivity of the system to changes of boundary conditions, giving information on the extension of eigenstates [11, 12]. In the transfer matrix description,

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the localization properties are controlled by the eigenvalues of $T(E)$ [4, 5]. The transfer matrix is also a useful tool in the scattering problem, where the disordered part has a finite length and is connected to infinite leads that carry plane waves. The matrix elements provide the transmission and reflection amplitudes that, in the Landauer approach, are related to transport properties of the single specimen [4].

The presence of statistical disorder implies the introduction of an ensemble of Hamiltonians, and the definition of average quantities, like the energy density, or the Lyapounov exponent for the resulting ensemble of transfer matrices. A relation, named after Thouless, relates the average Lyapounov exponent, which describes the localization length of eigenvectors in infinitely long wires, to the energy density [13].

In the transition to higher dimensions, or by allowing hopping to occur among sites inside a finite range, the Jacobi structure of the Hamiltonians of these systems is often preserved, with the matrix elements being replaced by square matrices. The aim of this work is to study in a general framework the properties of Hamiltonians with tridiagonal block structure, and those of the related transfer matrices, in the cases of periodic or scattering boundary conditions. However, the random character of such Hamiltonians, whose description requires the notion of ensemble, is not considered here: the properties of a single general matrix with the tridiagonal block structure are investigated.

The Schrödinger equation $\mathcal{H}\psi(t) = \mathrm{i}\partial_t\psi(t)$ is considered with the following Hamiltonian,

$$(\mathcal{H}\psi)_n = L_{n-1}^{\dagger}\psi_{n-1} + H_n\psi_n + L_n\psi_{n+1} \tag{1.4}$$

where H_n and L_n are complex matrices of size M, with the only requirement $H_n = H_n^{\dagger}$ and $\det L_n \neq 0$. The Hamiltonian is then a block-Jacobi matrix, with diagonal blocks H_n, upper and lower adjacent blocks L_n and $L_n^{\dagger}$.

The matrices H_n describe a transverse or internal dynamics, and the L_n couple adjacent transverse sections, aligned in one direction. In the Anderson model on a hypercubic lattice in $D+1$ dimensions, the matrices H_n have the structure of Anderson Hamiltonians in dimension D, and matrices $L_n = -I$ describe the coupling of nearest-neighbouring lattice slices [14]. A related disordered model with n orbitals per site was solved in the limit $n \to \infty$ [15]. In band random matrices, the H_n are GOE or GUE random matrices, and the L_n are lower triangular random matrices [16]. In a similar model for mesoscopic fluctuations, the L_n are square random matrices [17, 18].

The content of the paper is as follows. In section 2 a conservation law is obtained from the eigenvalue equation, which plays an essential role in the theory, and will be interpreted as current conservation in the scattering problem. The transfer matrix is then introduced, together with the definition of the velocity matrix. For completeness, in section 3 we briefly discuss the Hamiltonian for a finite chain. Of greater interest is the periodic chain, discussed in section 4, where an identity involving the spectra of the periodic Hamiltonian and of the transfer matrix is found, which allows a detailed analysis of the band structure. Section 5 is devoted to the study of the scattering problem. In particular, the role of the velocity matrix and of closed channels is discussed in the construction of the transfer matrix for current amplitudes. The main results are summarized in the conclusions, section 6.

2. The basic tools

2.1. A conservation law

The eigenvalue equation for $\mathcal{H}$, written in block form and with a real energy value E,

$$L_{n-1}^{\dagger}\psi_{n-1} + H_n\psi_n + L_n\psi_{n+1} = E\psi_n \tag{2.1}$$

leads to a conservation law of local type, with interesting consequences. By taking the scalar product with ψ_n we obtain the relation

$$\psi_n^{\dagger}L_{n-1}^{\dagger}\psi_{n-1} + \psi_n^{\dagger}L_n\psi_{n+1} = \psi_n^{\dagger}(E - H_n)\psi_n$$

with a real right-hand side. Therefore, $0 = \mathrm{Im}(\psi_n^{\dagger}L_{n-1}^{\dagger}\psi_{n-1} - \psi_{n+1}^{\dagger}L_n\psi_n)$, which implies that $\mathrm{Im}(\psi_{n+1}^{\dagger}L_n^{\dagger}\psi_n)$ does not depend on n. Explicitly, up to a factor, this quantity is

$$\mathcal{C} = -\mathrm{i}\Psi_n^{\dagger}\Sigma_n\Psi_n \tag{2.2}$$

where we have introduced a compound vector that suits the transfer matrix approach, and a matrix related to the longitudinal dynamics:

$$\Psi_n = \begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} \qquad \Sigma_n = \begin{pmatrix} 0 & L_n^{\dagger} \\ -L_n & 0 \end{pmatrix}. \tag{2.3}$$

2.2. The transfer matrix

The eigenvalue equation (2.1) has the structure of a two-term recurrence relation for the vectors ψ_n into which ψ is partitioned, and becomes single term in the compound notation

$$\Psi_n = T_n(E)\Psi_{n-1} \tag{2.4a}$$

where we introduce the one-step transfer matrix, $T_n(E)$, of size $2M$

$$T_n(E) = \begin{pmatrix} L_n^{-1}(E - H_n) & -L_n^{-1}L_{n-1}^{\dagger} \\ I & 0 \end{pmatrix} \tag{2.4b}$$

with the property, which follows from the conservation law,

$$T_n(E)^{\dagger}\Sigma_n T_n(E) = \Sigma_{n-1}. \tag{2.5}$$

Note that this property, which is derived quite naturally in the block approach, would not easily show in the case of a one-dimensional system while considering the transfer process between subsequent sites [19]. It is the block approach that efficiently takes into account the symmetry property of the Hamiltonian.

By iterating the transfer process, one constructs a N-step transfer matrix, with reference to an initial site:

$$\Psi_N = T(E)\Psi_0 \qquad T(E) = T_N(E)T_{N-1}(E)\ldots T_1(E). \tag{2.6a}$$

The matrix $T(E)$ is a polynomial of degree N in the energy parameter E, and for any value it satisfies the relation

$$T(E)^{\dagger}\Sigma_N T(E) = \Sigma_0 \tag{2.6b}$$

which imposes constraints on the matrix coefficients; in particular, the determinant is independent of E.

The case $\Sigma_0 = \Sigma_N$ corresponds to interesting situations that may be of physical relevance: the chain of finite length, the periodic chain and the scattering problem, which

will be discussed in the next sections. At this stage, it is important to explore the general spectral properties of matrices of size $2M$ that satisfy the relation

$$T^\dagger \Sigma T = \Sigma \tag{2.7}$$

with the matrix Σ having the properties $\Sigma^\dagger = -\Sigma$, $\det \Sigma \neq 0$.

Such matrices form a group, with $T^{-1} = \Sigma^{-1} T^\dagger \Sigma$. If Φ is an eigenvector of T with eigenvalue z, then $\Sigma\Phi$ is an eigenvector of $T^\dagger$, with eigenvalue $1/z$. Therefore, both z and $1/z^*$ belong to the spectrum of T. From equation (2.7) we obtain

$$(\Phi_i^\dagger \Sigma \Phi_j)(z_i^* z_j - 1) = 0. \tag{2.8}$$

This relation describes a property of an important matrix of the theory, which is now introduced.

2.3. The velocity matrix

Let Z be the diagonal matrix of eigenvalues z_i of T, which in general consist of ρ complex pairs ξ, $1/\xi^*$, with $|\xi| < 1$, and 2ν numbers on the complex unit circle, with $\rho + \nu = M$. The feature of having an even number of eigenvalues on the unit circle, which follows just by counting, is important for the discussion of the bands or the scattering problem. Let us choose the following partitioning into four subsets:

$$\mathrm{e}^{\mathrm{i}p_1} \dots \mathrm{e}^{\mathrm{i}p_\nu} \qquad \xi_1 \dots \xi_\rho \qquad \mathrm{e}^{\mathrm{i}p'_1} \dots \mathrm{e}^{\mathrm{i}p'_\nu} \qquad \frac{1}{\xi_1^*} \dots \frac{1}{\xi_\rho^*}. \tag{2.9}$$

At this level, the pairing and priming of phases is arbitrary. Let U be the corresponding matrix whose columns are the eigenvectors Φ_i of T, so that

$$T = U Z U^{-1}. \tag{2.10}$$

The spectral decomposition and the property (2.7) allow us to introduce a Hermitian matrix Ω, which is significant for the applications,

$$\Omega = -\mathrm{i} U^\dagger \Sigma U \tag{2.11}$$

with the following property, that corresponds to equation (2.8),

$$Z^\dagger \Omega Z = \Omega. \tag{2.12}$$

Since Z is diagonal, most of the matrix elements in Ω vanish: $\Omega_{ij}(z_i z_j^* - 1) = 0$. The pattern of the matrix depends on the ordering of the eigenvalues in Z. With the choice (2.9) we obtain

$$\Omega = \begin{pmatrix} V & \gamma \\ \gamma^\dagger & V' \end{pmatrix} \tag{2.13a}$$

where the blocks V, V' and γ are diagonal matrices of size M, with main diagonals

$$V = \{v_1 \dots v_\nu, 0 \dots 0\} \qquad V' = \{v'_1 \dots v'_\nu, 0 \dots 0\} \qquad \gamma = \{0 \dots 0, \gamma_1 \dots \gamma_\rho\}. \tag{2.13b}$$

For future use, we specify the non-zero matrix elements:

$$v_i = -\mathrm{i}\Phi_i^\dagger \Sigma \Phi_i \qquad v'_i = -\mathrm{i}\Phi_{M+i}^\dagger \Sigma \Phi_{M+i} \qquad i = 1 \dots \nu \tag{2.14a}$$

$$\gamma_i = -\mathrm{i}\Phi_{\nu+i}^\dagger \Sigma \Phi_{M+\nu+i} \qquad i = 1 \dots \rho. \tag{2.14b}$$

The eigenvalues of Ω are the ν pairs of real numbers v_i, v'_i and the 2ρ numbers $\pm|\gamma_j|$. By Sylvester's law of inertia [20], the matrix Ω has the same signature, defined as the difference

of the numbers of positive and negative eigenvalues, as the Hermitian matrix $-\mathrm{i}\Sigma$. For a matrix Σ with the structure (2.3), the eigenvalues of $-\mathrm{i}\Sigma$ solve.

$$\det(s + \mathrm{i}\Sigma) = \det(s^2 - L^\dagger L) = 0. \tag{2.15}$$

They are $\pm s_i$, where s_i^2 are the M eigenvalues of the positive Hermitian matrix $L^\dagger L$. Therefore, the signature both of $-\mathrm{i}\Sigma$ and Ω is zero. The distinction between unprimed and primed phases in the diagonal of Z (2.9) is such that the former correspond to $v_i > 0$ and the latter correspond to $v_i' < 0$. These 2ν positive and negative values will be interpreted as velocities, and Ω will be named the velocity matrix. A pairing criterion for the phases p_i and p_i' will be given in the discussion of the band structure of periodic Hamiltonians.

3. The finite chain

For completeness, and to gain some insight into the structure of the transfer matrix, we briefly consider the case of a Hamiltonian matrix of finite size. The chain of finite length N corresponds to the boundary conditions $\psi_0 = 0$ and $\psi_{N+1} = 0$ in the eigenvalue equation (2.1). The transfer matrix for the chain $T(E) = T_N(E)T_{N-1}(E)\dots T_1(E)$ is constructed by setting $L_N = L_0 = I$ in its first and last matrix factors, which gives the property

$$T(E)^\dagger \sigma_2 T(E) = \sigma_2 \qquad \sigma_2 = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}. \tag{3.1}$$

In the transfer matrix approach, $\{\psi_n\}_{n=1}^N$ is an eigenvector with eigenvalue E of the matrix $\mathcal{H}$ if

$$\begin{pmatrix} 0 \\ \psi_N \end{pmatrix} = T(E) \begin{pmatrix} \psi_1 \\ 0 \end{pmatrix} \qquad T(E) = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \tag{3.2}$$

which means that ψ_1 is an eigenvector of the block $T(E)_{11}$, of size M, with eigenvalue 0. Therefore, $\det[E - \mathcal{H}] = 0$ whenever $\det T(E)_{11} = 0$. More precisely, since both determinants are polynomials in E of degree NM with the same roots, one can write

$$\det T(E)_{11} = \det[L_1 \dots L_{N-1}]^{-1} \det[E - \mathcal{H}]. \tag{3.3}$$

By construction, besides $T(E)_{11} = \{T_N \dots T_1\}_{11}$, we have $T_{21} = \{T_{N-1} \dots T_1\}_{11}$, $T_{12} = -L_1^{-1}L_0^\dagger\{T_N T_{N-1} \dots T_2\}_{11}$ and $T_{22} = -L_1^{-1}L_0^\dagger\{T_{N-1} \dots T_2\}_{11}$. Therefore T_{12}, T_{21} and T_{22} are polynomial matrices in E of degree $N-1$, $N-1$ and $N-2$, respectively.

4. The periodic chain

To investigate the connection between the spectrum of the transfer matrix and the spectrum of the Hamiltonian, one must consider the interesting case of periodic Hamiltonian, with period N: $L_{n+N} = L_n$, $H_{n+N} = H_n$.

By Bloch's construction, the spectral problem for $\mathcal{H}$ corresponds to that of a family of matrices, parametrized by a continuous parameter $p \in [-\pi, \pi]$. The procedure is the following: since the Hamiltonian commutes with the N-block shift operator, we look for eigenvectors of $\mathcal{H}$ which are also eigenvectors of the shift operator

$$\psi_{n+N} = \mathrm{e}^{\mathrm{i}p}\psi_n \qquad -\pi \leqslant p \leqslant \pi. \tag{4.1}$$

In applications, the requirement of periodicity corresponds to the topology of a ring, and the phase change (4.1) corresponds to a magnetic flux through it, measured by the Bloch parameter p.

Choosing an origin, for each value of p, the eigenvalue equation (2.1) with the above constraint corresponds to that of the following matrix, with $z = e^{ip}$, incorporating the boundary condition implied by (4.1):

$$\mathcal{H}(z) = \begin{pmatrix} H_1 & L_1 & 0 & \dots & & 0 & (1/z)L_N^\dagger \\ L_1^\dagger & H_2 & L_2 & 0 & & & 0 \\ 0 & L_2^\dagger & H_3 & L_3 & 0 & & \\ & 0 & \dots & & & & \\ & & & & \dots & L_{N-2} & 0 \\ 0 & & & 0 & L_{N-2}^\dagger & H_{N-1} & L_{N-1} \\ zL_N & 0 & & & 0 & L_{N-1}^\dagger & H_N \end{pmatrix}. \tag{4.2a}$$

By introducing $\mathcal{H}_0$, the matrix with corners removed, and $\mathcal{L}$, the matrix with the lower left corner equal to the block L_N, we also write

$$\mathcal{H}(z) = \mathcal{H}_0 + z\mathcal{L} + \frac{1}{z}\mathcal{L}^\dagger. \tag{4.2b}$$

It is useful to let both z and E be complex numbers. We construct the following transfer matrix:

$$T(E) = \begin{pmatrix} L_N^{-1}(E - H_N) & -L_N^{-1}L_{N-1}^\dagger \\ I & 0 \end{pmatrix} \dots \begin{pmatrix} L_1^{-1}(E - H_1) & -L_1^{-1}L_N^\dagger \\ I & 0 \end{pmatrix} \tag{4.3}$$

with the property

$$T(E^*)^\dagger \Sigma T(E) = \Sigma \qquad \Sigma = \begin{pmatrix} 0 & L_N^\dagger \\ -L_N & 0 \end{pmatrix}. \tag{4.4}$$

When E is complex, if z is an eigenvalue of $T(E)$, $1/z^*$ is an eigenvalue of $T(E^*)$.

4.1. The dual identities

We now derive the identities between the characteristic equations of the matrix $\mathcal{H}(z)$ and of the transfer matrix $T(E)$.

A N-block column vector $\psi = \{\psi_n\}_{n=1}^N$ is an eigenvector of $\mathcal{H}(z)$ with eigenvalue E if and only if

$$\begin{pmatrix} \psi_{N+1} \\ \psi_N \end{pmatrix} = T(E) \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} \begin{cases} \psi_{N+1} = z\psi_1 \\ \psi_0 = (1/z)\psi_N. \end{cases} \tag{4.5}$$

This means that z is an eigenvalue of $T(E)$, with eigenvector Φ of block components ψ_1 and ψ_0. We, therefore, have the dual relation

$$\det[E - \mathcal{H}(z)] = 0 \quad \leftrightarrow \quad \det[T(E) - z] = 0. \tag{4.6}$$

The relation can be turned into an equality by noting: (i) the characteristic polynomial $\det[E - \mathcal{H}(z)]$ has degree NM in the variable E with coefficient of the highest power equal to one; (ii) though the transfer matrix $T(E)$ has size $2M$, and is obtained as a product of N matrices linear in E, it can be shown by induction that $\det[T(E) - z]$ is a polynomial of degree NM in E, with the following coefficient of the highest power in E:

$$(-z)^M \det[L_N \dots L_1]^{-1}. \tag{4.7}$$

One can, therefore, write the interesting identity

$$\det[T(E) - z] = (-z)^M \det[L_N \dots L_1]^{-1} \det[E - \mathcal{H}(z)]. \tag{4.8a}$$

In this relation we substitute E and z with E^* and z^*, and take the complex conjugate. Noting that, by equation (4.4), $T(E^*)^\dagger$ is similar to $T(E)^{-1}$, and $\mathcal{H}(z^*)^\dagger = \mathcal{H}(1/z)$, we obtain

$$\det[T(E)^{-1} - z] = (-z)^M \det[L_N^\dagger \dots L_1^\dagger]^{-1} \det[E - \mathcal{H}(1/z)]. \tag{4.8b}$$

Taking the product of determinants (4.8a, b), we obtain a relation which is valuable for discussing the band structure of the periodic Hamiltonian:

$$\det\left[T(E) + T(E)^{-1} - \left(z + \frac{1}{z}\right)\right] = \prod_{k=1}^{N} |\det L_k|^{-2} \det[E - \mathcal{H}(z)] \det\left[E - \mathcal{H}\left(\frac{1}{z}\right)\right]. \tag{4.8c}$$

The two determinants in the right-hand side are coincident in the particular but important cases of periodic and antiperiodic boundary conditions $z = \pm 1$. They always coincide when the matrices H_n and L_n are real, since in this case $\mathcal{H}(1/z) = \mathcal{H}(z)^t$.

The equation generalizes the result (1.3), contained in [7, 10] for Jacobi matrices, $M = 1$. For this case, in the appendix, a useful formula for level velocities is given.

4.2. Level dynamics

The NM eigenvalues of $\mathcal{H}(z)$ are functions of the parameter z whose derivatives have interesting applications [21–23]. The first derivative is the level velocity, measuring the current in the ring problem, or being the group velocity in the scattering problem. The second derivative is the curvature. In this section it is shown that the first derivative, when the eigenvalue $E(z)$ is real, is an entry of the velocity matrix.

If E is an eigenvalue of $\mathcal{H}(z)$, E^* is an eigenvalue of $\mathcal{H}(1/z^*)$, since one matrix is the Hermitian conjugate of the other. Let us write the eigenvalue equations

$$\mathcal{H}(z)\psi = E\psi \qquad \mathcal{H}(1/z^*)\tilde{\psi} = E^*\tilde{\psi} \tag{4.9}$$

with eigenvectors $\psi = \{\psi_n\}_{n=1}^N$ and $\tilde{\psi} = \{\tilde{\psi}_n\}_{n=1}^N$. We take the logarithmic derivative of the first equation

$$\left(z\mathcal{L} - \frac{1}{z}\mathcal{L}^\dagger\right)\psi + \mathcal{H}(z) z \frac{\mathrm{d}}{\mathrm{d}z}\psi = z\frac{\mathrm{d}E}{\mathrm{d}z}\psi + E(z) z \frac{\mathrm{d}}{\mathrm{d}z}\psi$$

and multiply on the left by $\tilde{\psi}^\dagger$. Using the second eigenvalue equation we obtain

$$z\frac{\mathrm{d}E}{\mathrm{d}z}(\tilde{\psi}^\dagger\psi) = \tilde{\psi}^\dagger\left(z\mathcal{L} - \frac{1}{z}\mathcal{L}^\dagger\right)\psi. \tag{4.10}$$

Let us normalize to one the scalar product in the left-hand side. Due to the simple structure of the matrix $\mathcal{L}$, the right-hand side simplifies to

$$z\tilde{\psi}_N^\dagger L_N \psi_1 - \frac{1}{z}\tilde{\psi}_1^\dagger L_N^\dagger \psi_N.$$

Using the boundary conditions $\psi_N = z\psi_0$, $\tilde{\psi}_N = (1/z^*)\tilde{\psi}_0$, and denoting by Φ the eigenvector of $T(E)$ with eigenvalue z, of components ψ_1 and ψ_0, and by $\tilde{\Phi}$ the eigenvector of $T(E^*)$ with eigenvalue $1/z^*$, of components $\tilde{\psi}_1$ and $\tilde{\psi}_0$, we obtain

$$z\frac{\mathrm{d}E}{\mathrm{d}z} = \tilde{\psi}_0^\dagger L_N \psi_1 - \tilde{\psi}_1^\dagger L_N^\dagger \psi_0 = -\tilde{\Phi}^\dagger \Sigma \Phi. \tag{4.11}$$

For a real value of the energy, we recognize the non-zero matrix elements of the velocity matrix (2.14).

In the case $z = e^{ip}$, the matrices $\mathcal{H}(e^{ip})$ and $\mathcal{H}(e^{-ip})$ are Hermitian and each have NM real eigenvalues, respectively, described by functions $E_j(p)$ and $E_j(-p)$ spanning the same set of NM energy bands, as p varies in $[-\pi, \pi]$.

Given an energy value E inside a band of label j, recall that the transfer matrix $T(E)$ admits at least one pair of eigenvalues on the unit circle, e^{ip} and $e^{ip'}$, such that both $\mathcal{H}(e^{ip})$ and $\mathcal{H}(e^{ip'})$ have the eigenvalue E: $E_j(p) = E_j(p') = E$, respectively, yielding a positive and a negative velocity

$$\frac{dE_j}{dp}(p) = -i\Phi_j^\dagger \Sigma \Phi_j = v_j \qquad \frac{dE_j}{dp}(p') = -i\Phi_{j+M} \Sigma \Phi_{j+M} = v'_j. \tag{4.12}$$

The velocities describe the istantaneous speeds by which, in E, the band j is covered in the two directions. The appearance of 2ν eigenvalues on the unit circle corresponds to the overlapping in E of ν bands. These properties are now discussed with the help of the dual identities.

4.3. Band structure of the spectrum

The dual identities (4.8) provide the connection among the eigenvalues of Hamiltonian matrices and transfer matrices: if E is an eigenvalue of $\mathcal{H}(z)$, z is an eigenvalue of $T(E)$ and $z + 1/z$ is an eigenvalue of $T(E) + T(E)^{-1}$. The latter eigenvalues are useful for the determination of the band structure of the spectrum of the periodic Hamiltonian.

Taking into account the results of section 2, when E is real, the matrix $T(E)+T(E)^{-1} = U(Z + Z^{-1})U^{-1}$ has eigenvalues

$$\begin{cases} \lambda_j(E) = 2\cos p \quad \lambda_{j+M}(E) = 2\cos p' & j = 1 \dots \nu \\ \lambda_{\nu+j}(E) = \xi_j + \xi_j^{-1} = \lambda_{\nu+j+M}(E)^* & j = 1 \dots \rho. \end{cases} \tag{4.13}$$

If $\lambda_j(E) = 2\cos p$ and $1 \leqslant j \leqslant \nu$, E is an eigenvalue of $\mathcal{H}(e^{ip})$ with positive velocity v_j. On the other hand, there is also a value p' such that E is an eigenvalue of $\mathcal{H}(e^{ip'})$, since both phases appear in the spectrum of $T(E)$. Then, since the latter phase involves a negative velocity, there is an eigenvalue $\lambda_{j+M}(E) = 2\cos p'$ with negative velocity v_{j+M}. The structure of bands is determined by the behaviour of these pairs of eigenvalues, as is now discussed.

It is convenient to plot the functions $\lambda_j(E)$ in the E–λ plane. When $z = e^{ip}$, both matrices $\mathcal{H}(z)$ and $\mathcal{H}(1/z)$ are Hermitian and have NM real eigenvalues $E_i(p)$ and $E_i(-p)$. This implies that the line $\lambda = 2\cos p$ must, for any p, have $2NM$ intersections with the graphs of the functions $\lambda_j(E)$. None of such functions can have an extremum inside the strip $|\lambda| < 2$, because this would violate the existence of $2NM$ intersections for all p.

The strip is then crossed by $2NM$ lines that correspond to portions of the graphs of an even number of functions $\lambda_j(E)$.

On the other hand, from the knowledge of the properties of $T(E)$, if E is any eigenvalue, it is the projection on the E axis of at least one pair of points, given by the intersections of the pair of lines $\lambda = \lambda_j(E)$ and $\lambda = \lambda_{j+M}(E)$, respectively, with $\lambda = 2\cos p$ and $\lambda = 2\cos p'$. The number of intersections may be greater than two, but always even.

When $p = 0$ or $p = \pm\pi$, the eigenvalues of the matrices $\mathcal{H}(e^{ip})$ and $\mathcal{H}(e^{-ip})$ are coincident. The NM pairs of lines $\lambda = \lambda_j(E)$ and $\lambda = \lambda_{j+M}(E)$, when reaching from below the upper border of the strip $\lambda = 2$, join at the NM points whose abscissae are the NM eigenvalues of $\mathcal{H}(1)$. The same pairs join when reaching from above the lower border $\lambda = -2$, in points of abscissa given by the eigenvalues of $\mathcal{H}(-1)$. Between these extrema, each pair λ_j and λ_{j+M} forms a loop whose projection on the E axis determines a band.

The equations determining the bands produced by the pair of eigenvalues λ_j and λ_{j+M} are two, providing different dynamics for the eigenvalues of $\mathcal{H}(e^{ip})$:

$$2\cos p = \lambda_j(E(p)) \quad p \in \mathcal{I}_{\pm} \qquad 2\cos p = \lambda_{j+M}(E(p)) \quad p \in \mathcal{I}_{\mp} \tag{4.14}$$

where $\mathcal{I}_+$ is the interval $0 \leqslant p \leqslant \pi$, and $\mathcal{I}_-$ is the interval $-\pi \leqslant p \leqslant 0$, and the upper sign occurs for $\lambda_j'(E) \leqslant 0$. The velocities are then respectively positive and negative:

$$\frac{\mathrm{d}E(p)}{\mathrm{d}p} = -2\sin p \left(\frac{\mathrm{d}\lambda_j}{\mathrm{d}E}\right)^{-1}_{E=E(p)} \qquad \frac{\mathrm{d}E(p)}{\mathrm{d}p} = -2\sin p \left(\frac{\mathrm{d}\lambda_{j+M}}{\mathrm{d}E}\right)^{-1}_{E=E(p)}. \tag{4.15}$$

This discussion shows that the eigenvalues of $T(E)$ on the unit circle, as functions of E, are naturally paired. This follows from the pairing of the eigenvalues of $T(E)+T(E)^{-1}$ in the strip $|\lambda| \leqslant 2$ which is determined by the band structure of the energy. The pairing can be traced out of the strip, since they become complex conjugated, until eventually re-entering the strip at a common point.

The case where $T(E)$ is real is considerably simpler, since $p' = -p$. Then, the lines (4.14) coincide, and velocities for $p > 0$ and $p < 0$ are opposite.

5. The scattering problem

In a scattering problem, the scattering region is confined to a set of blocks $n = 1 \ldots N$, outside which we assume, with enough generality, that the infinite matrix $\mathcal{H}$ has a constant structure.

$$\begin{array}{ccccccccccc}
\ldots & \ldots & L_0 & & & & & & & & \\
 & L_0^\dagger & H_0 & L_0 & & & & & & & \\
 & & L_0^\dagger & H_0 & L_0 & & & & & & \\
 & & & L_0^\dagger & H_1 & L_1 & & & & & \\
 & & & & L_1^\dagger & H_2 & \ldots & & & & \\
 & & & & \ldots & \ldots & L_{N-1} & & & & \\
 & & & & & L_{N-1}^\dagger & H_N & L_0 & & & \\
 & & & & & & L_0^\dagger & H_0 & L_0 & & \\
 & & & & & & & L_0^\dagger & H_0 & \ldots. &
\end{array} \tag{5.1}$$

The two infinite tails, which model the 'leads', must sustain propagating states which enable us to construct ingoing and outgoing scattering states. Such states, solutions of the eigenvalue equation (2.1) in the left- and right-hand sides of the scatterer, are connected by the transfer matrix for the scatterer $T(E) = T_N(E) \ldots T_1(E)$. The matrix depends on the coupling to the free dynamics, since it contains the matrix L_0 in its first and last factor. This dependence precisely endows the transfer matrix with the property, in general not shared by the single matrix factors,

$$T(E)^\dagger \Sigma_0 T(E) = \Sigma_0 \qquad \Sigma_0 = \begin{pmatrix} 0 & L_0^\dagger \\ -L_0 & 0 \end{pmatrix} \tag{5.2}$$

where Σ_0 is provided by the free part of the Hamiltonian, $\Sigma_0^\dagger = -\Sigma_0$ and $\det \Sigma_0 \neq 0$.

5.1. The free dynamics

The preliminary full understanding of the free dynamics is essential for the scattering problem. We shall find that, at a given energy, the number of open channels, corresponding to plane waves, is the same for the two directions of motion. In the basis of plane waves,

the velocity matrix replaces the matrix Σ_0, providing the interpretation of the law (2.2) as flux conservation.

Let us consider the Schrödinger equation with Hamiltonian $\mathcal{H}_0$, with scatterer removed and replaced by a sequence of H_0 and L_0 matrices:

$$L_0^\dagger \psi_{n-1}(t) + H_0 \psi_n(t) + L_0 \psi_{n+1}(t) = \mathrm{i}\partial_t \psi_n(t). \tag{5.3}$$

The general solution

$$\psi_n(t) = \sum_{j=1}^{M} \int_{-\pi}^{\pi} \mathrm{d}p\, c_j(p) u_j(p)\, \mathrm{e}^{\mathrm{i}\{np - E_j(p)t\}} \tag{5.4}$$

is a linear superposition of plane waves where $u_j(p)$ and $E_j(p)$ are provided by the eigenvalue problem of the Hermitian matrix, which is the particular case $N = 1$ of equation (4.2*b*):

$$\{H_0 + \mathrm{e}^{\mathrm{i}p} L_0 + \mathrm{e}^{-\mathrm{i}p} L_0^\dagger\} u_j(p) = E_j(p) u_j(p). \tag{5.5}$$

For any p there are M real energy values $E_j(p)$ which are distributed in M bands, and corresponding orthonormal eigenvectors $u_j(p)$. The bands may overlap, and together constitute the spectrum $\mathcal{S}$ of the free dynamics. The group velocity of a wave packet is given by

$$v_j(p) = \frac{\partial E_j(p)}{\partial p} = \mathrm{i} u_j(p)^\dagger (\mathrm{e}^{\mathrm{i}p} L_0 - \mathrm{e}^{-\mathrm{i}p} L_0^\dagger) u_j(p). \tag{5.6}$$

Since bands may overlap for a given allowed value E of the energy, there are in general $2\nu(E)$ values of momenta p_j and p_j', yielding positive and negative velocities, such that $E(p_j) = E(p_j') = E$. We call $\nu(E)$ the number of 'channels', which counts the number of propagating states with given energy, in one direction.

However, the transfer matrix approach, which is convenient for the scattering problem, involves solutions with fixed energy. The general solution (5.4) may be rewritten as

$$\psi_n(t) = \int_{\mathcal{S}} \mathrm{d}E\, \mathrm{e}^{-\mathrm{i}Et} \psi_n(E) \tag{5.7}$$

where $\psi_n(E)$ is a physical solution of

$$L_0^\dagger \psi_{n-1}(E) + H_0 \psi_n(E) + L_0 \psi_{n+1}(E) = E \psi_n(E) \tag{5.8a}$$

and, as such, in the two-vector formalism, is given by

$$\Psi_n(E) = T_0(E)^n \Psi_0 \tag{5.8b}$$

where Ψ_0 is a vector with a structure to be discussed later, that ensures the requirement of providing a 'physical solution', and $T_0(E)$ is the free transfer matrix evaluated at an admissible value of the energy $E \in \mathcal{S}$

$$T_0(E) = \begin{pmatrix} L_0^{-1}(E - H_0) & -L_0^{-1} L_0^\dagger \\ I & 0 \end{pmatrix}. \tag{5.9}$$

Besides physical states, there are also non-physical ones which, when the scatterer is included in the lattice, must be considered. We, therefore, study the spectral properties of $T_0(E)$. From

$$T_0(E)^\dagger \Sigma_0 T_0(E) = \Sigma_0 \tag{5.10}$$

we know that the spectrum of $T_0(E)$ contains ν pairs of non-zero eigenvalues $\mathrm{e}^{\mathrm{i}p_j}$ and $\mathrm{e}^{\mathrm{i}p_j'}$, and ρ complex pairs ξ_i and $1/\xi_i^*$, where $\nu + \rho = M$ and we assume $|\xi_i| < 1$.

Writing explicitly the eigenvalue equation for $T_0(E)$, one finds that the column eigenvector of $T_0(E)$, with eigenvalue z, has upper M components given by a vector zu and lower M components given by u, solution of the equation with fixed E

$$H(z)u = Eu \qquad H(z) = H_0 + zL_0 + z^{-1}L_0^\dagger. \tag{5.11}$$

In particular, we have the ν pairs of eigenvectors u_j and u'_j of equation (5.5), with eigenvalues e^{ip_j} and $e^{ip'_j}$. The remaining pairs ξ_i and $1/\xi_i^*$, with $|\xi_i| < 1$, have eigenvectors w_i and w'_i. From equation (5.11) and the reality of E, we immediately obtain the property that both $\xi_i(w_i^\dagger L_0 w_i)$ and $1/\xi_i^*(w_i'^\dagger L_0 w'_i)$ are real. Therefore, in the case $L_0 = L_0^\dagger$, the eigenvalues of $T_0(E)$ that are not on the unit circle, are real.

Let us introduce the ordering (2.9) of eigenvalues and eigenvectors. Then $T_0(E) = UZU^{-1}$ with

$$Z = \begin{pmatrix} Z_1 & 0 \\ 0 & Z_2 \end{pmatrix} \tag{5.12a}$$

$$Z_1 = \begin{pmatrix} e^{ip_1} & & & \\ & \cdots & & \\ & & e^{ip_\nu} & \\ & & & \cdots \\ & & & & \xi_\rho \end{pmatrix} \qquad Z_2 = \begin{pmatrix} e^{ip'_1} & & & \\ & \cdots & & \\ & & e^{ip'_\nu} & \\ & & & \cdots \\ & & & & 1/\xi_\rho^* \end{pmatrix} \tag{5.12b}$$

and U is the matrix of column eigenvectors, built from the eigenvectors of (5.11):

$$U = \begin{pmatrix} U_1 Z_1 & U_2 Z_2 \\ U_1 & U_2 \end{pmatrix} \qquad \begin{aligned} U_1 &= (u_1 \dots u_\nu, w_1 \dots w_\rho) \\ U_2 &= (u'_1 \dots u'_\nu, w'_1 \dots w'_\rho). \end{aligned} \tag{5.13}$$

The general solution of (5.8) is then

$$\psi_n(E) = \sum_{j=1}^{\nu} (a_j^{(\nu)} e^{ip_j n} u_j + b_j^{(\nu)} e^{ip'_j n} u'_j) + \sum_{j=1}^{\rho} (a_j^{(\rho)} \xi_j^n w_j + b_j^{(\rho)} (\xi_j^*)^{-n} w'_j). \tag{5.14}$$

The first sum involves physical states with positive and negative velocities, that contribute to propagation. The second sum is divergent for an unbounded chain, but once the scatterer is in place, it will provide exponential tails leaving the scatterer. In the compound notation, introducing a vector of $2M$ amplitues A, the solution (5.14) gains a compact form:

$$\Psi_n = UZ^n A \qquad A = \begin{pmatrix} a \\ b \end{pmatrix} \qquad a = \begin{pmatrix} a^{(\nu)} \\ a^{(\rho)} \end{pmatrix} \qquad b = \begin{pmatrix} b^{(\nu)} \\ b^{(\rho)} \end{pmatrix}. \tag{5.15}$$

From the spectral decomposition of the transfer matrix $T_0(E) = UZU^{-1}$, and the property (5.10) which also holds for powers of the transfer matrix, we construct the velocity matrix

$$\Omega_0 = -iU^\dagger \Sigma_0 U \qquad (Z^\dagger)^n \Omega_0 Z^n = \Omega_0. \tag{5.16}$$

The diagonal elements v_i and v'_i are precisely the positive and negative group velocities of the channels with momenta p_i and p'_i.

In the case that H_0 and L_0 are real matrices we have $p' = -p$, the energies are symmetric functions of the momentum $E_j(p) = E_j(-p)$, and accordingly $v_j = -v'_j$. This corresponds to the property of time-reversal invariance of the free dynamics. Note that $u'_j = u_j^*$, by taking the transposed of equation (5.5).

5.2. Current conservation

When the scatterer is included, the solutions of the eigenvalue equation (2.1) at the left and the right of the scatterer may contain a contribution that decays exponentially away from the scatterer. In the compound notation, the left and right solutions are of the type (5.15)

$$\Psi_n^{\mathrm{L}} = U Z^n A^{\mathrm{L}} \qquad A^{\mathrm{L}} = \begin{pmatrix} a \\ b \end{pmatrix} \qquad a^{(\rho)} = 0 \qquad n \leqslant 0 \tag{5.17a}$$

$$\Psi_m^{\mathrm{R}} = U Z^m A^{\mathrm{R}} \qquad A^{\mathrm{R}} = \begin{pmatrix} c \\ d \end{pmatrix} \qquad d^{(\rho)} = 0 \qquad m \geqslant N. \tag{5.17b}$$

The restrictions are needed to avoid the exponentially diverging parts, and are responsible for an interesting interpretation of the conservation law

$$(\Psi_n^{\mathrm{L}})^\dagger \Sigma_0 \Psi_n^{\mathrm{L}} = (\Psi_m^{\mathrm{R}})^\dagger \Sigma_0 \Psi_m^{\mathrm{R}}.$$

In terms of amplitudes they read

$$(A^{\mathrm{L}})^\dagger \Omega_0 A^{\mathrm{L}} = (A^{\mathrm{R}})^\dagger \Omega_0 A^{\mathrm{R}}. \tag{5.18}$$

Specifying the components, we obtain a law of current conservation, where no contribution comes from the non-propagating sector:

$$\sum_{j=1}^{\nu} (|a_j^{(\nu)}|^2 v_j + |b_j^{(\nu)}|^2 v_j') = \sum_{j=1}^{\nu} (|c_j^{(\nu)}|^2 v_j + |d_j^{(\nu)}|^2 v_j'). \tag{5.19}$$

The left and right vectors are related by the transfer matrix of the scatterer $\Psi_N^{\mathrm{R}} = T(E)\Psi_0^{\mathrm{L}}$. For the amplitudes we obtain the linear relation

$$A^{\mathrm{R}} = M(E) A^{\mathrm{L}} \qquad M(E) = Z^{-N} U^{-1} T(E) U \tag{5.20}$$

where both $M(E)$ and $U^{-1}T(E)U$ have the property

$$M(E)^\dagger \Omega_0 M(E) = \Omega_0. \tag{5.21}$$

5.3. The transmission and reflection matrices

Since some components in the amplitude vectors A^{R} and A^{L} have value zero and, moreover, we are not interested in the amplitudes of exponential tails, only a reduced transfer matrix is required for the computation of scattering quantities. Let us introduce the partitions

$$M(E) = \begin{pmatrix} M_1 & M_2 \\ M_3 & M_4 \end{pmatrix} \qquad M_k = \begin{pmatrix} M_k^{\nu\nu} & M_k^{\nu\rho} \\ M_k^{\rho\nu} & M_k^{\rho\rho} \end{pmatrix} \tag{5.22}$$

where, for example, $M_k^{\nu\nu}$ is the submatrix of size $\nu \times \nu$ of M_k. From the relation $A^{\mathrm{R}} = MA^{\mathrm{L}}$ we obtain the linear relation for the scattering components:

$$\begin{pmatrix} c^{(\nu)} \\ d^{(\nu)} \end{pmatrix} = M_S \begin{pmatrix} a^{(\nu)} \\ b^{(\nu)} \end{pmatrix}$$

$$M_S = \begin{pmatrix} M_1^{\nu\nu} - M_2^{\nu\rho}(M_4^{\rho\rho})^{-1} M_3^{\rho\nu} & M_2^{\nu\nu} - M_2^{\nu\rho}(M_4^{\rho\rho})^{-1} M_4^{\rho\nu} \\ M_3^{\nu\nu} - M_4^{\nu\rho}(M_4^{\rho\rho})^{-1} M_3^{\rho\nu} & M_4^{\nu\nu} - M_4^{\nu\rho}(M_4^{\rho\rho})^{-1} M_4^{\rho\nu} \end{pmatrix}. \tag{5.23}$$

If all channels are open, the matrix M_S coincides with M. As a consequence of equation (5.19), the matrix M_S has the property

$$M_S^\dagger \begin{pmatrix} v & 0 \\ 0 & v' \end{pmatrix} M_S = \begin{pmatrix} v & 0 \\ 0 & v' \end{pmatrix} \tag{5.24}$$

where v and v' are the diagonal matrices of the positive and negative velocities, respectively. The matrix blocks of M_S are directly related to the transmission matrix $\tilde{t}$ and the reflection matrix $\tilde{r}$ for amplitudes. In the scattering processes with incoming wave from the left and from the right respectively, we define

$$c^{(\nu)} = \tilde{t}^{\mathrm{L}} a^{(\nu)} \qquad d^{(\nu)} = 0 \qquad b^{(\nu)} = \tilde{r}^{\mathrm{L}} a^{(\nu)} \tag{5.25a}$$

$$c^{(\nu)} = \tilde{r}^{\mathrm{R}} d^{(\nu)} \qquad a^{(\nu)} = 0 \qquad b^{(\nu)} = \tilde{t}^{\mathrm{R}} d^{(\nu)}. \tag{5.25b}$$

To obtain a unitary scattering matrix, or define the conductance of the scatterer, one must consider the amplitudes of the incoming and outgoing fluxes in the various open channels, at the left and the right of the scatterer:

$$j_i^{\mathrm{in,L}} = a_i^{(\nu)} \sqrt{v_i} \qquad j_i^{\mathrm{out,L}} = b_i^{(\nu)} \sqrt{-v_i'}$$

$$j_i^{\mathrm{out,R}} = c_i^{(\nu)} \sqrt{v_i} \qquad j_i^{\mathrm{in,R}} = d_i^{(\nu)} \sqrt{-v_i'}. \tag{5.26}$$

The flux amplitudes are related by the transfer matrix

$$F = \Gamma M_S \Gamma^{-1} \qquad \Gamma = \begin{pmatrix} \sqrt{v} & 0 \\ 0 & \sqrt{-v'} \end{pmatrix} \tag{5.27a}$$

with the symplectic property corresponding to flux conservation

$$F^{\dagger} \sigma_3 F = \sigma_3 \qquad \sigma_3 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \tag{5.27b}$$

The matrix F is the canonical transfer matrix for the computation of transport quantities, like conductance [24, 25], since it takes into account the channel velocities and the possibility of closed channels.

From the matrix F one obtains the transmission and reflection matrices for flux amplitudes, which enter as blocks in a unitary scattering matrix, and are simply related to those for amplitudes (5.25)

$$t^{\mathrm{L}} = v^{-1/2} \tilde{t}^{\mathrm{L}} v^{1/2} \qquad r^{\mathrm{L}} = (-v')^{-1/2} \tilde{r}^{\mathrm{L}} v^{1/2} \tag{5.28a}$$

$$t^{\mathrm{R}} = (-v')^{-1/2} \tilde{t}^{\mathrm{R}} (-v')^{1/2} \qquad r^{\mathrm{R}} = v^{-1/2} \tilde{r}^{\mathrm{R}} (-v')^{1/2}. \tag{5.28b}$$

6. Conclusions

The motivation of this paper was to identify and study some basic ingredients common to many mathematical models for the description of quantum transport of a single particle in the presence of disorder. The process of ensemble average is usually a forward step that follows the identification of observable quantities that pertain to the single specimen. A single general Hamiltonian matrix with tridiagonal structure made of square blocks has therefore been considered. Some results of this paper, being very general, may also prove useful for other physical applications.

The relationship between the energy spectrum with the spectrum of the corresponding transfer matrix has been investigated, deriving 'dual identities' (4.8) among the characteristic polynomials of the two matrices, in the case of periodic boundary conditions, generalizing an identity known for the one-dimensional case [7, 10]. These relations allow the study of the band structure of the Hamiltonian and the level dynamics, which relates to observable quantities of the system, is relevant for the Thouless approach to conductance and, by taking ensemble average over disorder, have interesting universal properties for velocity correlations and curvatures [23]. It is hoped that the dual identities may be useful in the

study of the difficult and important problem of the statistical properties of transfer matrix eigenvalues, given those of the Hamiltonian.

It has been shown that, for closed, periodic or scattering boundary conditions, the transfer matrix of the whole chain has a generalized symplectic property, which generally does not hold for the single one-step factors of the transfer matrix. This property allows one to construct a Hermitean velocity matrix, with an even number of non-zero diagonal elements providing pairs of level velocities with opposite sign. In a scattering process they coincide with group velocities of wave packets travelling in opposite directions. The velocity matrix enters in the relation giving the generalized symplectic property for the transfer matrix for scattering amplitudes both for closed (non-propagating) and open channels. The procedure to restrict the transfer process to open channels only has been shown, in accordance with the usual scattering matrix approach.

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Appendix

When the blocks are not matrices but numbers ($M = 1$), we recover the usual Jacobi matrices of one-dimensional models. The transfer matrix is a 2×2 matrix. Letting the off-diagonal elements in the Hamiltonian be all equal to 1 for simplicity, the dual relation (4.8) with $z = \mathrm{e}^{\mathrm{i}p}$ gives equation (1.3), obtained by Last [7]. With simple steps, one can obtain the level velocities and the curvatures in the origin:

$$v_i(p) = \frac{\mathrm{d}E_i}{\mathrm{d}p} = -\frac{\sin p}{\prod_j'[E_i(p) - E_j(p)]}$$
$$K_i(0) = \frac{\mathrm{d}^2E_i}{\mathrm{d}p^2}(0) = -\frac{1}{\prod_j'[E_i(0) - E_j(0)]}. \tag{A.1}$$

The expression of curvature coincides with the product $\psi_1\psi_N$ of the first and last components of the eigenvector ψ of the matrix $\mathcal{H}(0)$ with energy E_i [12] and explains the meaning of curvature or of the bandwidth, to which curvature is related, as measures of localization [8].

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