



Figure 2: Dependence of the transmission coefficient with the incidence angle for two different kinds of designs of the FDM, with  $\eta = R$ ,  $n = 1$ , and: I)  $p = 3$ , and II)  $p = 2$  with reversed refraction indices.

the relationship between the resonant wavelengths and the QP structure of the substrate, and suggest the possibility of constructing resonating optical devices by properly matching the incidence angle of the incoming light with the size and design of the FDMs. Related work has been published elsewhere<sup>10</sup>.

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## Determination of Localization in Aperiodic Systems by using the Trace Map

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As a general trend, electronic localization in one dimensional systems with aperiodic hamiltonians is investigated by using the Lyapunov exponents of the wave-function. However, in this article we show that these exponents are usually used in a wrong way and thus they do not give information about localization. Here we propose a new way to investigate localization, which is based in the scaling of bands. This approach leads to consider the stability of a dynamical system, where the Lyapunov exponents of the trace map determine the localization. We also obtain a Thouless-type formula that is useful for quasiperiodic systems.

### 1. Introduction

In the study of localization properties of aperiodic hamiltonians, it is common to calculate the Lyapunov exponents (LE) of the wave-function in order to obtain a characteristic localization length<sup>1,2</sup>. To obtain these exponents, the formalism of the transfer matrix is usually utilized in 1D problems. However, most of the calculations of these exponents do not consider that the formal definition involves a limit from the right and from the left in the localization center<sup>3</sup>. Instead, the norm of the transfer matrix is taken, and the problem of the match between the solution from the left and from the right is not taken into account (this problem is known as the Borland paradox<sup>3</sup>). For critical states, this problem is even more difficult to tackle, and in this article, we show that the LE of an energy that is a solution of the Hamiltonian is zero, whatever the shape of the wave function. To avoid this problem, we propose an alternative definition that uses the scaling of the bands as a measure of localization. In this way, the problem of taken the limit from the left and from the right is avoided. Furthermore, the final result depends on the LE of the trace, taken in the sense of stability. This definition is very appropriate for quasiperiodic systems, since Kohmoto, Kadanoff and Tao<sup>4</sup> found a recurrence relation for the trace of a Fibonacci chain<sup>4</sup>. This relation defines a trace map, from which the spectrum can be found by successive iterations. After its introduction, this technique has produced many interesting results concerning the nature of the spectrum for diverse quasiperiodic systems, like the period-doubling<sup>5</sup> and Thue-Morse<sup>6</sup> chains. More recently, this formalism has been extended to aperiodic systems<sup>7</sup>. In this work, we also propose a variant of the Thouless formula<sup>8</sup>, which is useful for obtaining the characteristic exponent of localization for critical states.

## 2. Localization and stability of the trace

We consider the Schrödinger equation for a 1D tight-binding hamiltonian, defined on a chain of  $n$  sites, with an on-site potential  $V_n$  at site  $n$ , and hopping integral  $t$  between sites  $n$  and  $n + 1$ ,

$$t\psi_{n-1} + t\psi_{n+1} + V_n\psi_n = E\psi_n, \quad (1)$$

where  $\psi_n$  is the value of the wavefunction at site  $n$ . Eq.(1) can be rewritten in terms of the transfer matrix  $M(n)$  and a vector  $\Psi_n$  with components  $(\psi_n, \psi_{n-1})$ ,

$$\Psi_n \equiv \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} = \begin{pmatrix} (E - V_n)/t & -1 \\ 1 & 0 \end{pmatrix} \Psi_{n-1} \equiv M(n)\Psi_{n-1}. \quad (2)$$

A successive application of Eq. (2), gives the wave-function at site  $n$ , as a function of the value at the beginning of the chain,

$$\Psi_n = M(n)M(n-1)M(n-2)M(n-3)\dots M(2)\Psi_1 \equiv T(n)\Psi_1. \quad (3)$$

The allowed values for the energies are those for which the norm of trace of the matrix  $(\tau_n \equiv \text{tr}T(n))$  is less than two<sup>8</sup>. To determine the localization of an state, usually the Lyapunov exponents are used. They are defined as<sup>8</sup>,

$$\gamma(E) = \lim_{n \rightarrow \infty} \frac{1}{n} \log |\lambda_{\max}|, \quad (4)$$

where the greatest eigenvalue of the transfer matrix is denoted by  $\lambda_{\max}$ . We can obtain the maximum eigenvalue of  $T(n)$  by using the characteristic equation of the transfer matrix,

$$\det(\lambda - T(n)) = \lambda^2 - \lambda\tau_n + 1 = 0, \quad (5)$$

where we used that the determinant of the transfer matrix is one, since it is the product of matrices with determinant one, and that the trace is an invariant under unitary transformations. By solving Eq.(5) we found the two eigenvalues of  $T(n)$ ,

$$\lambda_{\pm} = \frac{\tau_n \pm \sqrt{\tau_n^2 - 4}}{2}. \quad (6)$$

For energies which satisfies  $\|\tau_n\| > 2$ , the eigenvalues are real and the LE are,

$$\gamma(E) = \lim_{n \rightarrow \infty} \frac{1}{n} \log (|\tau_n| + \sqrt{\tau_n^2 - 4}). \quad (7)$$

Inside the spectrum  $\|\tau_n\| \leq 2$ ,  $\lambda_{\pm}$  are complex, both with unitary norm, and thus the LE is zero, since  $\|\tau_n\|$  is always 1. Thus, they do not give information about localization for energies that are eigenvalues of the problem. In order to surmount this problem, we can relate localization with the scaling of bands. We start by considering a piece of system of size  $n$ , that can be amorphous, quasiperiodic or periodic. Using this portion of the system as a unit cell, we can construct an infinite crystal by joining the cells side by side.

The resultant crystal has Bloch solutions and a band spectrum. However, the bandwidth is determined by the wave-function overlap at the border of the cells. For exponentially localized states in the unit cell  $n$ , the bandwidth of the crystal is  $W_n \sim \langle \psi_1 | H | \psi_2 \rangle \sim t_n e^{-\xi}$ , where  $\langle \psi_1 |$  and  $\psi_2 \rangle$  are two similar eigenstates in contiguous cells, and  $\xi$  is the localization length. A similar calculation for extended states shows that the bandwidth do not depend on  $n$ . For critical states,  $W_n \sim n^{-\beta(E)}$ . Using these relations, we can define a characteristic exponent for critical states as,

$$\beta_n(E) = \log(W_n)/\log(n). \quad (8)$$

The bandwidth can be obtained from the trace since the band edges are the points where  $\tau(E) = \pm 2$ . In a previous work<sup>9</sup>, it was used a Taylor expansion in order to get an approximation for the localization length from the trace. However, in this work we show an exact result. We start by writing the following polynomial as,

$$\tau_n(E) - 2 = \prod_{i=1}^n (E - E_i), \quad (9)$$

where  $E_i$  are the roots of  $\tau_n(E) - 2 = 0$ . After taking the logarithm of the derivative evaluated in one of the band edges ( $E_s$ ) we get,

$$\log \left( \frac{d\tau_n(E)}{dE} \right)_{E=E_s} = \sum_{i \neq s} \log(E_s - E_i). \quad (10)$$

Using that  $E_i$  are the only values that satisfies a cyclic boundary condition for the cell of size  $n$  (in other words,  $E_i$  is an eigenvalue of the finite system), and dividing by  $n$ , we can use the density of states  $(\rho_n(E))$  of the unit cell to perform the sum. This leads to the Thouless formula<sup>3</sup> for the inverse of the localization length  $\xi(E_s)$ , but this time we get an expression that depends on the trace,

$$\frac{1}{n} \log \left( \frac{d\tau_n(E)}{dE} \right)_{E=E_s} = \int_{-\infty}^{\infty} \rho_n(E') \log(E_s - E') dE' \equiv \frac{1}{\xi(E_s)}. \quad (11)$$

For quasiperiodic systems, instead of dividing by  $n$ , we divide by  $\log(n)$  in order to obtain a value different from zero, and thus we get a modified type of Thouless formula that is appropriate for quasiperiodic systems since it gives the scaling exponent of the wave-function,

$$\beta_n(E_s) = \frac{1}{\ln n} \log \left( \frac{d\tau_n(E)}{dE} \right)_{E=E_s} = \frac{n}{\ln n} \int_{-\infty}^{\infty} \rho_n(E') \log(E_s - E') dE'. \quad (12)$$

Eq. (11) and (12) characterize the localization properties of the wave-function. However, if we write the derivative of the trace with respect to  $E_s$  as follows,

$$\frac{1}{\xi(E_s)} = \frac{1}{n} \lim_{\epsilon \rightarrow 0} \log \left( \frac{\tau_n(E_s + \epsilon) - \tau_n(E_s)}{\epsilon} \right).$$

we observe that this expression corresponds exactly to the LE of the trace map, used in the sense of dynamical systems, i.e., it measures how the trajectories of the trace diverges as the initial conditions are changed by  $\epsilon$ . Furthermore,

since  $E_j$  is a band edge, we can conclude that the properties of localization are determined by the stability of the trace map around the point  $\tau_n(E) = 2$ . This is clearly related with the scaling of bands. When we have a localized state, the bands shrink in an exponential way as the system grows, and thus the band edges also shrink. For example, if for a certain generation we have  $\tau_n(E_j) = 2$ , for the next generations the trace evaluated at the same energy must be outside the band,  $\tau_{n+N}(E_j) > 2$ . Thus, a localized state corresponds to a repulsive fixed point of the trace, since the LE of the trace is greater than zero.

The former stability approach has several consequences in the trace map, where the trace of a certain length is a function of the trace of previous lengths,

$$\tau_n(E_j) = f(\tau_{n-1}(E_j), \tau_{n-2}(E_j), \dots, \tau_1(E_j)).$$

Extended states are those for which  $\tau_n(E_j) = \pm 2$  for any  $n$  and fixed  $E_j$ . Thus,  $\pm 2$  is a hyperbolic fixed point of the trace map. In quasiperiodic systems, usually the bands are subdivided as  $n$  grows since the spectrum is a type of Cantor set. Thus, the number of points  $E_j$  grows with the system size, and the trace map must be non-linear. As an example, we can consider the trace map of the Fibonacci chain,

$$\tau_{F(n)}(E) = \tau_{F(n-1)}(E)\tau_{F(n-2)}(E) - \tau_{F(n-3)}(E),$$

where  $F(n)$  is the  $n$ -esim Fibonacci number. Clearly, the point  $\tau_{F(n-1)}(E) = \tau_{F(n-2)}(E) = \tau_{F(n-3)}(E) = 2$  is a fixed point. Due to the non-linear character of the map, the number of band edges grows with the system size.

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## Delone Covering of Canonical Tilings $\mathcal{T}^*(D_6)$

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We consider canonical quasiperiodic tiling projected from a lattice  $\mathcal{T}^*(D_6)$  whose window in perpendicular space is projected Voronoi cell,  $V_L$ , and whose tiles in parallel space are projected boundaries of Delone cells,  $X_L^*$ , six golden tetrahedra. The tiles are coded by corresponding dual Voronoi boundaries projected to  $\mathbb{E}_L$ , denoted by  $X_L$ . We try to obtain the Delone covering of the tiling by projecting to the parallel space some of the Delone cells ( $D^h$ ,  $h = a, c, b$ ) of the  $D_6$  lattice. We determine the coding in orthogonal space for these Delone clusters and their fillings by the tiles. The covering of the tiling by the corresponding Delone clusters is considered.

### 1. Delone Clusters and Windows of $\mathcal{T}^L$

The quasilattice points, the vertices of the tiles  $X_L^*$  in a canonical tiling  $\mathcal{T}^*(L)$  are those lattice points  $q \in L$ , projected to  $\mathbb{E}_L$  ( $q_L$ ), such that  $q_L \in V_L$ . The vertices of the windows for the tiles,  $X_L$ , are the holes  $h$  of the lattice  $L$ .

We project to the parallel space  $\mathbb{E}_L$  those Delone cells  $D^h$  from  $L$  whose projection  $D_L^h$  is a union of projected tiles  $X_L^*$ , such that it covers  $D_L^h$  exactly and forms a patch of the tiling without gaps and overlaps<sup>1,2,3</sup>. The patch we call Delone cluster  $D_L^h$ .

The coding in  $\mathbb{E}_L$  of the Delone cluster, its window, is the coding of the patch in the tiling which fills  $D_L^h$  completely. The generating code  $w(h)$  of the window of  $D_L^h$  is a coding of the patch which enforces the filling of the cluster by the tiles  $X_L^*$ .

The window of  $D_L^h$  turns out to be the finite set of the polytopes congruent to the generating code<sup>4,5</sup>. They are in the window of the tiling,  $V_L$  (to  $\mathbb{E}_L$  projected Voronoi cell) translated with respect to each other and all attached to the hole positions of type  $h$ .

In the tiling  $\mathcal{T}^*(D_6)$ , the filling of the Delone clusters is unique<sup>2</sup>, up to the (projecting) symmetry.

### 2. Delone Covering of the Tiling $\mathcal{T}^*(D_6)$

The window of the canonical tiling  $\mathcal{T}^*(D_6)$  is a triacontahedron of standard 5fold edge length  $\odot = 1/\sqrt{2}$ .  $V_L = \mathcal{T}^{\odot}$ . The tiles are 6 golden tetrahedra ( $X_L^* = C_L^*$ ,  $F_L^*$ ,  $A_L^*$ ,  $B_L^*$ ,  $D_L^*$ ,  $C_L^*$ ) of 2fold edge lengths  $\ominus = \sqrt{2}/(\tau + 2)$  and  $\tau \ominus$ . The