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Wave-Function Scaling Exponents and the Trace Map of a Fibonacci Chain

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Approximate analytical expressions for the scaling exponents of the electronic wave-function of a Fibonacci chain are obtained from the trace map. This is done by relating the stability of the trace map with the localization nature of the system. A comparison is made with the only state for which an analytical expression of the scaling exponent is known.

Keywords Quasicrystals; aperiodic Hamiltonian; critical states; trace map

1. Introduction

After the discovery of quasicrystals, the Fibonacci chain (FC) and the Harper model have been widely used as benchmark tools to understand the effects of quasiperiodicity [1]. For the FC, it has been proved that the spectrum is singular continuous (fractal), with critical wave-functions [2]. In higher dimensions (D), the nature of the spectrum and the localization properties are not well understood, due to the different topology [3]. Even in 1D it has not been possible to find the scaling properties and the effects of the boundary conditions for all the eigen-functions, although now there are many well developed mathematical techniques to study quasiperiodic Hamiltonians [4]. Only for a certain state of the FC the exact scaling exponent of the wave-function is known, and as we will see, some discrepancies in its value appear in the literature [5–7]. Part of the problem resides in the failure of the usual tools to investigate localization. To solve this, an alternative approach has been proposed by the author [8]. In 1D, this approach turned out to be closely connected with the nature of the transfer matrix trace map renormalization group flow, which usually was used to determine the spectrum (set of allowed electron energies). In this article, we present new analytical results for the scaling exponents and the nature of localization in a quasiperiodic system, using the trace map renormalization group and the method published previously [8].

2. Scaling Exponents and the Trace Map

As a model, we use a Hamiltonian defined on a chain of n sites, with a potential V_n at site n, and hopping integral t_{n+1} between sites n and $n+1$. The corresponding Schröedinger equation is, $t_n\psi_{n-1} + t_{n+1}\psi_{n+1} = (E - V_n)\psi_n$, where ψ_n is the value of the wavefunction at site n, and E is the energy. This equation can be rewritten in terms of the transfer matrix

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$M_n(E)$, and a vector $\Psi(n)$ with components (ψ_n,ψ_{n-1}), such that $\Psi(n+1)=M_n(E)\Psi(n)$. The wave-function at site n is given by a successive application of the previous relation,

$$\Psi(n+1) = M_n(E)M_{n-1}(E)\ldots M_1(E)\Psi(1) = T_n(E)\Psi(1).$$

The spectrum is the set of energies for which the trace norm $\tau_n(E) \equiv trT(n,E)$ is less [2] than 2. For many systems, there are recurrence relations of the trace [5] as a function of the trace of m smaller chains of lengths l_j of the form $\tau_n(E) = \mathrm{f}(\tau_{l_{n-1}}(E),\tau_{l_{n-2}}(E),\ldots,\tau_{l_1}(E))$. These types of relations are called trace maps. In a previous work [8], we showed that the properties of localization are determined by the stability of the map around the points $\tau_n(E) = \pm 2$, since for a rational approximant, the bandwidths are determined by the wave-function overlap. Localized states correspond to repulsive fixed points of the map [8]. For extended states, the bands edges (energies that we denote by E_s) do not change with the system size, and thus $\tau_n(E_s) = \pm 2$, is a fixed point of the trace map [8], *i.e.*, the map must satisfy $\pm 2 = \mathrm{f}(\pm 2, \pm 2, \pm 2, \ldots)$, where the point is hyperbolic in nature [8]. In 1D quasiperiodic systems, the bands of the approximants are subdivided as n grows, and thus the number of points E_s also grows with the system size. For quasiperiodic systems, the wave-function decays as [2] $\psi_n \approx n^{\beta_n(E)}$. Hence, for a rational approximant with a unit cell size of length n, the bandwidth scales as: $W_n(E) \approx < \psi_n|\mathrm{H}|\psi_{n+1} > \approx t_n n^{2\beta_n(E)}$. Since $W_n(E)$ is determined by the trace, it can be proved that [8],

$$\beta_n(E) = \frac{1}{2\ln(n)} \ln\left(\frac{d\tau_n(E)}{dE}\right) \tag{1}$$

The scaling exponent obtained from this equation is a minimum, since the wavefunction overlap between the unitary cells of a rational approximant is dominated by the maximal overlap. This is the most important exponent, because it rules the maximum conductivity of the system. If the gaps between the bands are very small compared with W_n, corrections may appear due to hybridization of levels in neighboring cells. Now we will use this technique for studying the FC, which is a Hamiltonian with two kinds of atoms, A and B arranged in a Fibonacci sequence. The trace of a FC with length $F(l)$ ($F(l)$ is the Fibonacci number of generation l) is given by [5],

$$x_l(E) = x_{l-1}(E)x_{l-2}(E) - x_{l-3}(E), \tag{2}$$

where $x_l(E) = \tau_n(E)/2$. The map has as initial conditions [5], $x_{-1}(E) = 1$, $x_0(E) = (\mathrm{E} - \lambda)/2$ and , $x_1(E) = (\mathrm{E} + \lambda)/2$, where $\lambda = |\,(\mathrm{V}_A - V_B)|/2$ in the diagonal case. For the off-diagonal case $\lambda = |\delta - (1/\delta)|/2$, where $\delta = t_A/t_B$.wheret_A and t_B are the hopping integrals between atoms A and B. The nature of the states can be deduced from the approach presented. First we obtain the fixed points of the map (x^*). From Eq. (2), $x^* = 2(x^*)^2 - x^*$. Two solutions are found, $x^* = 0$ and $x^* = 1$. The first solution is not consistent with the initial conditions, since the map has an invariant manifold [5]. From the invariant, is easy to show that the other fixed point, $x^* = 1$, occurs only when we have a periodic chain, $\lambda = 0$ and $V(n) = V_A = V_B$. For this value of λ, the system presents extended states, but is instructive to apply the method presented to determine localization. In principle, from the fact that there are fixed points of the map for $\lambda = 0$, this means that the states are localized or extended. Now we investigate the nature of the stability around $x^*(E) = 1$ by making a linearization of the equations. The map can be seen as a trajectory [5] in 3D of the point $(\mathrm{x}_{n+1}, \mathrm{x}_n, \mathrm{x}_{n-1})$. Since the map is a vectorial function, the derivative is a 3×3 matrix, and

when we move around the fixed point P by the small vector $\mathrm{dP} = (\varepsilon_x, \varepsilon_y, \varepsilon_Z)$, we obtain,

$$\begin{pmatrix} x_{n+2}(\mathrm{P}+\mathrm{dP}) \\ x_{n+1}(\mathrm{P}+\mathrm{dP}) \\ x_n(\mathrm{P}+\mathrm{dP}) \end{pmatrix} = \begin{pmatrix} x_{n+2}(\mathrm{P}) \\ x_{n+1}(\mathrm{P}) \\ x_n(\mathrm{P}) \end{pmatrix} + \begin{pmatrix} 2x_l(\mathrm{P}) & 2x_{l+1}(\mathrm{P}) & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \end{pmatrix}$$

The stability nature is obtained from the eigenvalues of the matrix evaluated at the point $\boldsymbol{p} = (1, 1, 1)$; these eigenvalues are $\mathrm{r}_1 = -1$, $\mathrm{r}_2 = \sigma^2$, $\mathrm{r}_3 = 1/\sigma^2$, where $\sigma = (\sqrt{5}+1)/2$. Since $\mathrm{r}_2 > 1$ and $\mathrm{r}_3 < 1$, the point is hyperbolic. The hyperbolic nature of the flux means that the states are extended. There are not repulsive fixed points, hence localized states are not observed. The other possibility is to have critical states when $\lambda \neq 0$, as it is revealed from the fact that the map contains two cycles [6]: one of period 2 and the other with period 6. From this, one can show that the trace scales as $\tau_{l+6}(E) = (\tau_l(E))^{\alpha(E)}$. Using Eq. (1), the stability of the map predicts that the scaling exponent of the wave-function is,

$$\beta(E) = \alpha(E)/2 \tag{3}$$

For example, at $E = 0$ the bandwidth is dominated by the 6 cycle [6]. An stability analysis can be made, except that now the derivative is obtained by multiplying the matrices in each point of the cycle. The resulting matrix eigenvalues are [6],

$$r_1 = -1, \quad r_{2,3} = [(1 + 4(1 + \lambda^2)^2)^{1/2} \pm 2(1 + \lambda^2)]^2$$

and the scaling exponent of the trace is $\alpha(0) = \ln \sigma^6 / \ln \mathrm{r}_2 \cdot E = 0$ is the only state for which an analytical expression is known [6]. Later on, a different result for the same state was published [7], and two limiting exponents were obtained, one is a maximum and the other a minimum [7]. In Fig. 1, a comparison between these works and ours, given by Eq. (3) is shown. For $\delta \gg 1$, all the results coincide (and also for $\delta \ll 1$, due to the symmetrical form of λ with respect to t_A and t_B). For $\delta \to 1$, the obtained exponent deviates from the

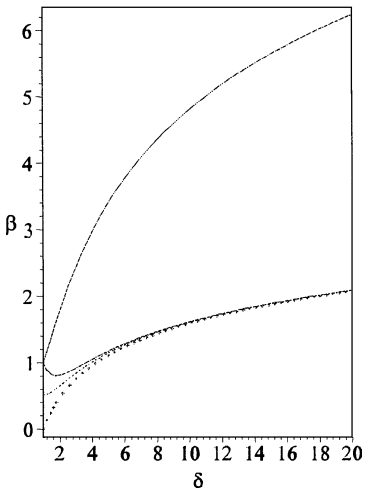

FIGURE 1 Scaling exponents for $E = 0$. The dashed line was obtained using the method of this work. Crosses (lower curve) are obtained form Kohmoto et al. [6]. The solid lines (upper curves) are from Fujiwara et al. [7].

previously published results [6, 7]. However, it has been proved that for this state, β depends on the boundary conditions [9, 10]. To improve the results for $\delta \to 1$, the hybridization of levels needs to be taken into account, as we will show in future works.

In conclusion, we showed how the FC trace map can be used to determine the scaling exponents of the critical wave-functions and the nature of localization.

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