Electronic transport in the Koch fractal lattice

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In this work we extend the algebraic approach introduced in the context of general Fibonacci systems [E. Maciá and F. Domínguez-Adame, Phys. Rev. Lett. **76**, 2957 (1996)] to analytically study the transmission coefficient of a subset of states in the fractal Koch lattice. We report on the existence of extended states whose transmission coefficients periodically oscillate as the Koch curve approaches its fractal limit.
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I. INTRODUCTION

Prior to the discovery of quasicrystals it was suggested by Rammal that fractal structures, which instead of the standard translation symmetry exhibit *scale invariance*, may be suitable candidates to bridge the gap between crystalline and disordered materials.[1] Such a possibility was further elaborated by Schwalm's work on inhomogeneous fractal glasses,[2] a class of structures which are characterized by a scaling distribution of pore sizes and a great variety in the site environments. On the other hand, the unexpected finding of quasicrystalline alloys exhibiting forbidden crystallographic symmetries, was originally thought as corresponding to a phase intermediate between a crystal and a liquid,[3] but subsequently interpreted as a natural extension of the notion of a crystal to structures with *quasiperiodic*, rather than periodic, translational order.[4] From this perspective it is interesting to compare the physical properties related to these two representatives of the orderings of matter, namely, quasicrystals and fractals.

Albeit both kinds of structures possess peculiar electronic spectra supported by Cantor sets of zero Lebesgue measure,[1,5] it has been pointed out that electron dynamics on fractal substrates are *richer* than those encountered in quasiperiodic structures such as the Fibonacci chain.[6] Thus, for example, localized, critical, and extended wave functions alternate in a complicated way in several fractal models,[7] while it is known that all allowed states in Fibonacci chains are critical.[8] Consequently, the general question as to whether certain specific features of the states might be induced by the fractality of the substrate becomes pertinent. Dealing with the frequency spectrum, it has been reported that the interplay between the local symmetry and the self-similar nature of a fractal gives rise to the existence of persistent superlocalized modes.[9] This class of states, introduced by Lévy and Souillard,[10] arises as a consequence that the minimum path between two points on a fractal does not always follow a straight line. In this article, we will further illustrate the richness of fractal spectra by showing the existence of *transparent* electronic states in fractal lattices.

To address this topic we shall consider the tight-binding model on the Koch lattice introduced by Andrade and Schellnhuber (AS).[11] The motivation for this choice stems from the fact that this model Hamiltonian can be exactly mapped onto a linear chain, and the corresponding electron dynamics expressed in terms of just two kinds of transfer matrices. In this way we are able to extend the algebraic approach recently introduced to analytically study general Fibonacci systems[12] to describe a fractal system as well.

II. THE MODEL

Let us start with a brief description of the model sketched in Fig. 1. The corresponding tight-binding Hamiltonian is given by[11]

$$H=\sum_n \{|n\rangle\langle n+1|+|n\rangle\langle n-1|+\lambda f(n)[|n-1\rangle\langle n+1| + |n+1\rangle\langle n-1|]\},$$

where λ is the cross-hopping integral introduced by Gefen[13] [indicated by dashed lines in Fig. 1(a)] and

$$f(n)=\delta(0,n)+\sum_s^{k-1} \delta\left(\frac{4^s}{2},n(\mathrm{mod}4^s)\right),$$

with $k\geqslant 2$ and $-4^k/2\leqslant n\leqslant 4^k/2$, describes the effective next-nearest-neighbor interaction in the kth stage of the fractal growth process. Our model differs from that studied by AS

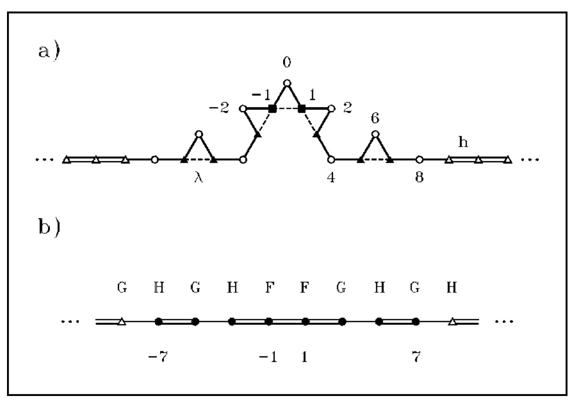

FIG. 1. (a) sketch of the Koch lattice considered in this work, (b) sketch of the renormalization scheme mapping the Koch lattice into a linear chain.

in the fact that we are considering a *finite* fractal lattice embedded in an infinite periodic arrangement of identical sites connected by hopping integrals h. The main effect of allowing electron hopping across the folded lattice is the existence of sites with different coordination numbers along the lattice, a characteristic feature of fractals which is not shared by quasiperiodic lattices. Depending on the value of their respective coordination numbers we can distinguish twofold (circles), threefold (full triangles), and fourfold (squares) sites. We then notice that even sites are always twofold, a fact which allows us to renormalize the original lattice[11] mapping it into the linear form sketched in Fig. 1(b). The hopping integrals represented by single bonds appear always isolated from one another. The hopping integrals represented by double bonds can appear either isolated or forming trimers. Consequently, there are three possible site environments in the renormalized Koch lattice which, in turn, define three possible types of transfer matrices, labeled F, G, and H in Fig. 1(b). Now, by introducing the matrices[11] $A \equiv HG$ and $AB \equiv FF$, it can be shown by induction that the global transfer matrix at any given arbitrary stage k of the fractal growth process M_k can be iteratively related to that corresponding to the previous stage M_{k-1} by the expression

$$A^{-1}M_k = M_{k-1}^2 B M_{k-1}^2, \tag{1}$$

with $k \geqslant 2$ and $M_1 \equiv A$. Note that Eq. (1) slightly differs from the expression given by AS since we are considering a finite system instead of a periodic approximation. At this point the parallelism between the AS approach and the transfer matrix renormalization technique intruced by us[12] becomes apparent. In fact, both approaches are able to translate the topological order of the lattice to the transfer matrices sequence describing the electron dynamics in a natural way.

III. SPECTRUM AND TRANSMISSION COEFFICIENTS

We will now focus on two algebraic properties of the matrices A and B which allow us to perform an *analytical* study of a subset of the wave functions belonging to the Koch lattice spectrum. On the one side, we realize that both matrices are *unimodular* (i.e., their determinant equals unity) for *any* choice of λ *and* for *any* value of the electron energy E. In addition, they commute for certain values of the energy. In fact, after some algebra we get

$$[A,B] = a(\lambda,E)\begin{pmatrix} (2-E^2)r & r^2 \\ (1-E^2)(E^2-3) & (E^2-2)r \end{pmatrix}, \tag{2}$$

where $r \equiv 1 + \lambda E$,

$$a(\lambda,E) \equiv \frac{\lambda E(E^2-2)(2+\lambda E)}{r^3}, \tag{3}$$

and we have defined the origin of energies in such a way that the hopping integrals along the chain equal unity. The commutator (2) vanishes in four different cases. (i) The choice $\lambda = 0$ reduces the original Koch lattice to a trivial periodic chain, so that all the allowed states, $-2 \leqslant E \leqslant 2$, are extended. (ii) The center of the energy spectrum $E=0$. The extended nature of this state was shown by AS.[11] (iii) $E = \pm\sqrt{2}$. (iv) The family of states satisfying $E = -2/\lambda$. For these energies the condition $[A,B]=0$ is fulfilled and, making use of the Cayley-Hamilton theorem for unimodular matrices,[14] the global transfer matrix of the system, $M_k \equiv A^{n_A}B^{n_B}$, with $n_A = 4^{k-1}+1$, and $n_B = 4^{k-2}+1$, can be explicitly evaluated in terms of Chebyshev polynomials of the second kind. From the knowledge of M_k the condition for the considered energy value to be in the spectrum, $|\mathrm{Tr}[M_k]| \leqslant 2$, can be readily checked and, afterwards, its transmission coefficient can be determined explicitly. In this way we uncover a subset of the Koch lattice energy spectrum whose eigenstates can be studied analytically.

Let us consider, in the first place, the energies $E = \pm\sqrt{2}$. In this case we get

$$\mathrm{Tr}[M_k] = -\frac{1}{(1 \pm \sqrt{2}\lambda)^{n_A-n_B}} - (1 \pm \sqrt{2}\lambda)^{n_A-n_B}. \tag{4}$$

A detailed study of the condition $|\mathrm{Tr}[M_k]| \leqslant 2$ in Eq. (4) indicates that the only allowed states correspond to $\lambda = \mp\sqrt{2}$, for which $\mathrm{Tr}M_k = -2$. Consequently, these states are just two particular cases of the more general family (iv) which we shall discuss next.

By taking $E = -2/\lambda$ we get $B = -I$, where I is the identity matrix, so that $M_k = -A^{n_A}$. According to Cayley-Hamilton theorem we can express the global transfer matrix as

$$M_k = U_{n_A-2}(x)I - U_{n_A-1}(x)A, \tag{5}$$

where $U_m(x) \equiv \sin[(m+1)\theta]/\sin\theta$, with $x \equiv \mathrm{Tr}A/2 \equiv \cos\theta = -(\lambda^4 - 8\lambda^2 + 8)/\lambda^4$, are Chebyshev polynomials of the second kind. Therefore, making use of the relationship $U_{m+1} - 2\cos\theta U_m + U_{m-1} = 0$, the global transfer matrix corresponding to the energies $E = -2/\lambda$ can be expressed in the closed form

$$M_k = \begin{pmatrix} U_m - U_{m+1} & -q(\lambda)U_m \\ q(\lambda)U_m & U_{m-1} - U_m \end{pmatrix}, \tag{6}$$

where $q(\lambda) \equiv 2(\lambda^2-2)/\lambda^2$, $m \equiv n_A - 1$, and we must keep in mind that the condition $|\cos\theta| \leqslant 1$ implies $|\lambda| \geqslant 1$. From expression (6) we get $\mathrm{Tr}[M_k] = -2\cos\alpha$, where $\alpha \equiv n_A\theta$, and, consequently, we can ensure that these energies belong to the spectrum in the fractal limit ($k \to \infty$). Now, we calculate the transmission coefficient t, a magnitude directly related to the Landauer resistivity,[15] ρ, by embedding the Koch lattice in an infinite periodic arrangement as indicated in Fig. 1(a). In this way we obtain

$$t(k,\lambda) = \frac{1}{1+\rho} = \frac{1}{1 + \{[\lambda(\lambda \pm 2)/2(\lambda \pm 1)]\sin\alpha(k,\lambda)\}^2}, \tag{7}$$

where the plus (minus) sign in the factor of $\sin\alpha$ corresponds to the choices $h \equiv 1$ and $h \equiv r = -1$, respectively, for the hopping integral of the periodic leads. Several conclusions can be drawn from this expression. We must recall that the states can be classified, depending on the value of its related transmission coefficient, in *transparent* states with $t=1$, *localized* states with $t=0$, and *critical* states with $0 < t \leqslant 1$. This classification takes into account that, in addition to the Bloch states present in crystalline, periodic systems, the notion of transparent state must be widened to include electronic states which are not Bloch functions, such as those found in Fibonacci quasiperiodic systems.[12] Keeping this in mind, from expression (7) we realize that the transmission coefficients corresponding to the family (iv) are always bounded below for *any* stage of the fractal growth process, which proves their *extended* nature in the fractal limit. In addition, the choices $\lambda=\pm 2$ ($E=\mp 1$) correspond to states which are transparent at every stage of the fractal growth process. A fact which ensures their *transparent* nature in the fractal limit as well. Furthermore, it is possible to find a number of cross-hopping integral values satisfying the transparency condition $t=1$ at certain stages of the fractal growth given by the condition $\alpha(k,\lambda)=p\pi$. Making use of the previous definitions for n_A and θ, the relationship between the fractal growth stage and the cross-hopping integral values satisfying the transparency condition can be explicitly expressed as

$$[1+\cos\beta(k)]\lambda^4-8\lambda^2+8=0, \tag{8}$$

where $\beta(k)\equiv p\pi/(4^{k-1}+1)$, and $-m\leqslant p\leqslant m$. After some rearrangements, and taking into account the trigonometrical identity

$$\sqrt{1\pm\sin\frac{\beta}{2}}=\cos\frac{\beta}{4}\pm\sin\frac{\beta}{4}, \tag{9}$$

the solutions of Eq. (8) can be expressed in the closed form

$$\lambda=\sec\left(\frac{\beta(k)+\pi}{4}\right). \tag{10}$$

In obtaining Eq. (10) we have restricted to the case $\lambda>0$ without loss of generality, since the phase diagram corresponding to the Koch system exhibits the symmetry $(E,\lambda)=(-E,-\lambda)$.[7] Expression (10) allows us to label the different transparent states at any given stage k, in terms of the integer p. For the particular choice $p=0$ we get $\lambda=\sqrt{2}$ at *every* step of the fractal growth, in agreement with our previous discussion of the state $E=-\sqrt{2}$.

IV. RESULTS AND DISCUSSION

In Fig. 2 we plot the transmission coefficient (7) at two successive stages $k=2$ and $k=3$, as a function of the cross-hopping value. In the first place, we note that the number of λ values supporting transparent states ν_λ progressively increases as the Koch curve evolves toward its fractal limit, according to the power law $\nu_\lambda=2(4^{k-1}+1)$. It is interesting to compare this figure with the number of sites, $N=4^k+1$, present at the stage k in the Koch lattice. Thus, we obtain $\nu_\lambda=(N+3)/2$, indicating that the number of Koch lattices able to support transparent states increases linearly with the system size and, consequently, that the fractal growth *favors* the presence of extended states in Koch lattices. In particular, we can state that, in the fractal limit, there exist an *infinitely numerable* set of cross-hopping integrals supporting transparent extended states in the Koch lattice.

Another general feature shown in Fig. 2 is the presence of a broad plateau around $\lambda=2$, where the transmission coefficients take values significatively close to unity. In addition, as λ separates from the plateau the local minima in the transmission coefficient $t_{\min}$ take on progressively decreasing values which tend to zero in the limits $\lambda\to\infty$ and $\lambda\to 1$. This behavior suggests that the *best* transport properties in the family (iv) should be expected for those states located around the plateau.

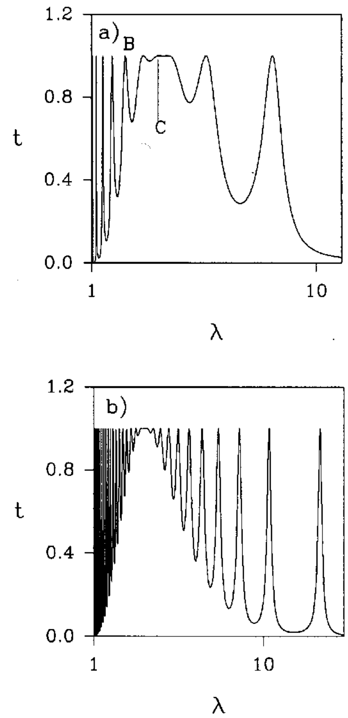

FIG. 2. Transmission coefficient as a function of the cross-hopping integral at two different stages (a) $k=2$, and (b) $k=3$. Peaks are labeled from left to right starting with $p=-4$ in (a). Label B corresponds to $p=0$. Label C indicates the transparent state at $\lambda=2$.

Up to now we have shown that, as the Koch lattice approaches its fractal limit, an increasing number of cross-hopping integrals are able to support transparent states in the $E=-2/\lambda$ branch of the phase diagram. In order to determine their related transport properties, we ask as to whether a state, whose transmission coefficient equals unity, at an arbitrary stage, say k, will prevail as a transparent state at the next stages of the fractal growth. From a detailed analysis of expression (7) we have found that the considered states can be classified into two separate classes. In the first class we have those states which are transparent at any stage k. In the second class we find states whose transmission coefficient *oscillates periodically* between $t=1$ and $t\equiv t_{\min}\neq 1$ depending on the value of k. Representative examples of such a behavior are provided in Fig. 3. Three general trends have been observed in this second class of extended states. In the first place, the values of $t_{\min}$ are significantly lower for states corresponding to $p<0$ than for states corresponding to $p>0$ (circles versus diamonds in Fig. 3). In the second place, at any given fractal stage, the values of $t_{\min}$ are substantially higher for states associated to cross-hopping integral values close to the plateau than for states corresponding to the remaining allowed λ values (an example corresponding to the

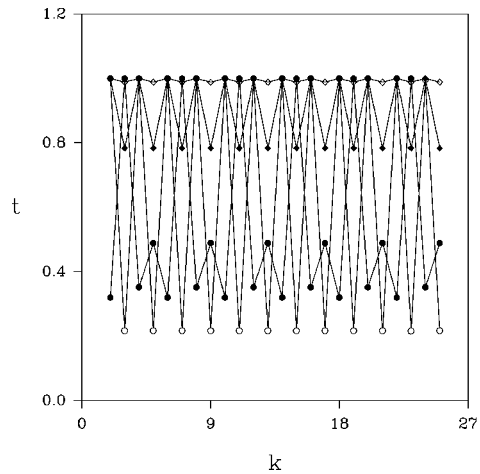

FIG. 3. Almost transparent states exhibiting periodic oscillations in their transmission coefficients as a function of k. Labeling key: (○) $p=-1$ in Fig. 2(a); (●) $p=-2$ in Fig. 2(b); (♦) $p=3$, in Fig. 2(a); (◇) $p=2$, in Fig. 2(a).

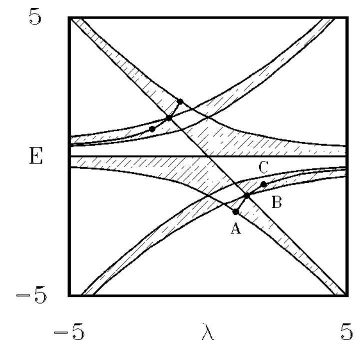

FIG. 4. Phase diagram showing the Koch lattice spectrum at $k=1$ (shadowed areas) and the branches corresponding to the extended states family $E=-2/\lambda$.

choice $p=2$ is shown for the state indicated by hollow diamonds in Fig. 3).

Therefore, we have found a class of extended electronic states whose transmission coefficients oscillate between $t=1$ and a limited range of $t_{\min}$ values depending on the value of the label integer p and the fractal growth stage. Consequently, we must consider the wave functions associated to the corresponding energies as representatives of extended states in the fractal limit, even though a definite value for the $t(k\rightarrow\infty,\lambda)$ does not exist. We tentatively will refer to these states as *almost transparent* ones and we expect their related transport properties to be more similar to that corresponding to usual transparent states than to localized ones. We must note, however, that not all these almost transparent states are expected to transport in much the same manner, as suggested by the diversity observed in the values of $t_{\min}$.

V. CONCLUSION

To conclude we will report on a general trend in the transport properties of electronic states belonging to family (iv). To this end, we refer to Fig. 4, where we provide a graphical account of the most relevant results presented in this work. In this figure we show the phase diagram corresponding to our model Hamiltonian at the first stage of the fractal process (shadowed landscape) along with two branches corresponding to the states belonging to the family $E=-2/\lambda$ (thick black lines). In the way along each symmetrical branch we find three particular states whose coordinates are respectively given by $(\pm 1,\mp 2)$, $(\pm\sqrt{2},\mp\sqrt{2})$, and $(\pm 2,\mp 1)$. Three of them, corresponding to the choice $\lambda>0$, are indicated by full circles labeled A, B, and C in Fig. 4. These states correspond to *transparent states* whose transmission coefficients equal unity *at every* stage k of the fractal growth. The remaining states in the branches correspond to *almost transparent* states exhibiting an oscillating behavior in their transmission coefficients. By comparing Figs. 2–4 we realize that the positions of the transparent states A,B,C allow us to define three different categories of almost transparent states according to their related transport properties. The first class (I) includes those states comprised between the state A, at the border of the spectrum, and the state B, located at a vertex point separating two broad regions of the phase diagram. The second class (II) includes those states comprised between the state B and the state C close to the plateau in the transmission coefficient around $\lambda=2$. Finally, the third class (III) comprises those states beyond the state C. The states exhibiting *better* transport properties belong to the classes II and III, and correspond to those states grouping around the plateau near the state C for which the values of $t_{\min}$ are very close to unity. As we move apart from state C, the transport properties of the corresponding almost transparent states become progresively worse, particularly for the states belonging to the class III, for which values of $t_{\min}$ as low as 10^{-3} can be found.

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