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LETTER TO THE EDITOR

On the existence of extended electronic states in a loopless fractal

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Abstract. It has been shown analytically that a proper tuning of the boundary condition can ensure an infinity of extended electronic eigenstates on a loopless semi-infinite Vicsek fractal. First we map this particular loopless fractal exactly onto a one-dimensional hierarchical chain. Within the framework of real space renormalization group and the transfer matrix methods we then demonstrate how a suitable choice of the on-site potential of an edge atom can generate a whole hierarchy of extended Bloch-like eigenfunctions.

The character of electronic eigenstates in one-dimensional lattices has always attracted the attention of condensed matter theorists. The periodicity or randomness in the distribution of on-site potentials on a chain of atoms is known to produce altogether different classes of electronic states. In the periodic case, the eigenstates are the Bloch functions, while in the presence of random disorder all the wavefunctions are localized in an exponential manner [1]. At the same time, it has also been established that disorder, in a deterministic way, may lead to the delocalization of electron wavefunctions, even in one dimension. The number of such delocalized (extended/resonance) wavefunctions may range from one [2] (in the case of a random dimer type model) to infinity [3] (in the case of a self-similar quasiperiodic chain of atoms). Such systems therefore provide examples of 1D systems where minibands of extended electronic states exist at special values of the electron energy in spite of the absence of any long-range translational symmetry.

In this letter we deal with another class of systems that do not have any translational order, namely fractals. We deal, in particular, with a loopless fractal lattice, called the Vicsek fractal, and we show that a proper choice of an edge atom in a semi-infinite Vicsek fractal can ensure the existence of an *infinite* number of extended electronic eigenstates. Our results are exact, and the method can be extended to other types of loopless fractal, though the tuning of the boundary atom may not be an essential criterion in all other cases.

Previous works on fractals have mainly been centred around the Sierpinski gasket (SG), which is a popular example of a fractal with loops. Electronic and harmonic excitations on a SG have already been studied in some detail. The general character of such spectra on this lattice turns out to be a Cantor set and the wavefunctions all localized for a gasket of infinite generation [4, 5]. Very recently, in an interesting piece of work, Kappertz and co-workers [6] studied the quantum dynamics of electrons on the non-branching Koch curve

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within the framework an exact real space renormalization scheme. A concise classification of the quantum states in a Koch curve has been presented.

Apart from these works, another interesting loopless fractal that has started receiving some attention in recent years is the well known Vicsek fractal [7–9]. Although a few studies about the nature of harmonic excitations on a Vicsek fractal are available in the literature [7–9], the electronic spectrum has practically remained unexamined. The only recent result, to the best of our knowledge, has been a calculation of the average density of states using a generating function approach [10], but this work does not shed any light on the nature of electronic eigenstates. In what follows, we now prove in a completely analytical way that a Vicsek fractal provides a very interesting example of a non-translationally invariant system, where a proper tuning of the site energy of an edge atom triggers an infinite number of Bloch-like electron eigenstates.

We describe the system by the usual tight-binding Hamiltonian for non-interacting electrons:

$$H = \sum_{n} \epsilon_n |n\rangle\langle n| + \sum_{\langle nm \rangle} t_{nm} |n\rangle\langle m| \tag{1}$$

where ϵ_n is the on-site potential at the nth atomic site and t_{nm} is the nearest-neighbour hopping integral. For a semi-infinite fractal, we assign a site energy ϵ_L to the extreme left atom. The other atoms at all the vertices have site energy ϵ_0. The nearest-neighbour hopping integral is kept uniform everywhere. It is easy to see (figure 1) that the entire fractal is built up by placing a basic five-site cluster side by side to form bigger clusters in higher generations. We now transform the fractal into a one-dimensional chain of atoms by decimating the upper and lower branches around a central site at any generation. This transformation is illustrated in figure 1 for a second-generation fractal. The semi-infinite effective 1D chain can now be easily constructed. It is interesting to find that the central sites in the original fractal are transformed into sites in the 1D chain with site energies ϵ_i, with $i = 1, 2, 3, \ldots$ distributed in a hierarchical way. Sequentially, the different values of ϵ_i arise out of decimations of bigger and bigger upper and lower clusters of atoms around the central sites at each scale of length. For example, the first such atom in the 1D chain has a site energy equal to $\epsilon_1 = \epsilon_0 + 2t^2/(E - \epsilon_0)$. The other site energies that create the hierarchical pattern in the transformed 1D lattice can be obtained in a similar fashion making use of the recursion relations provided in [9]. All other sites on the effective 1D chain have their site energies equal to ϵ_L and ϵ_0 corresponding to the extreme left atom and the other 'undecimated' atoms respectively.

We can now study the nature of electron states in this effective 1D chain in order to gain insight into the spectral character of the original Vicsek fractal. It is important to appreciate that the transformed chain and the parent fractal will support extended states, if there are any, at the same energy eigenvalues. We precisely adopt this line of attack, and show how a proper choice of the edge atom can lead to an infinity of extended electron states in the semi-infinite Vicsek fractal.

To prove the existence of such extended states at specified values of the energy, we need to solve the set of difference equations

$$(E - \epsilon_n)\psi_n = t\psi_{n+1} + t\psi_{n-1} \tag{2}$$

where ψ_n is the amplitude of the wavefunction on the nth atomic site and we have set the nearest-neighbour hopping integrals to be identical, and equal to t. It is easy to recast this equation in a matrix form

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = \begin{pmatrix} (E - \epsilon_n)/t & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}. \tag{3}$$

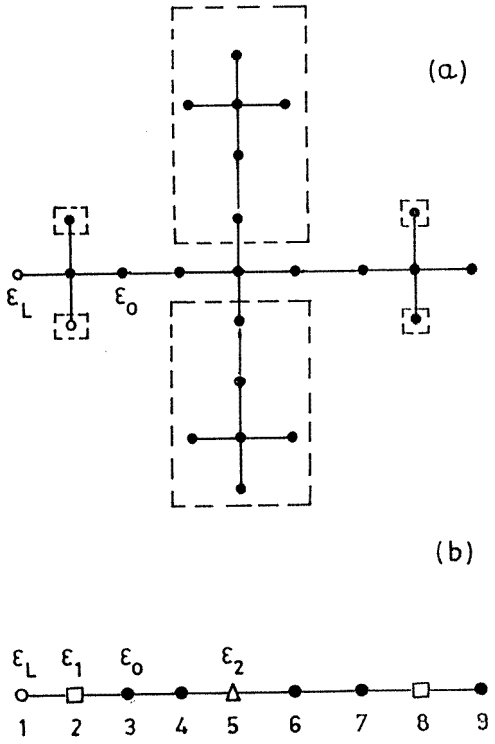

Figure 1. (a) A Vicsek fractal at its second generation. The sites that will be decimated are enclosed in 'dotted' boxes. (b) The transformed 1D chain. The edge site is marked with an open circle. Other sites are indicated by the solid circles, the square and the triangle.

The transfer matrix relating the amplitudes on the $(n+1)$th and nth site to those of the nth and $(n-1)$th site is a 2×2 unimodular matrix. Denoting such a matrix corresponding to the site with site energy ϵ_i by M_i and counting the sites from the left end, we observe that the amplitudes on the sixth and the fifth sites of the effective 1D chain can be written in terms of those of the third and the second sites as

$$\begin{pmatrix} \psi_6 \\ \psi_5 \end{pmatrix} = M_2 M_0 M_0 \begin{pmatrix} \psi_3 \\ \psi_2 \end{pmatrix}. \tag{4}$$

Noting the simple form of the individual transfer matrices it is possible to rewrite the above equation in the form [11]

$$\begin{pmatrix} \psi_6 \\ \psi_5 \end{pmatrix} = (I + \lambda_2 I_0) M_0^3 \begin{pmatrix} \psi_3 \\ \psi_2 \end{pmatrix}. \tag{5}$$

In the above equation I is the identity matrix, $I_0 = (\sigma_x + \mathrm{i}\sigma_y)/2$, and $\lambda_2 = (\epsilon_2 - \epsilon_0)/t$. σ_x and σ_y are the usual Pauli matrices.

Now, M_0 being a 2×2 unimodular matrix, we can write [12] $M_0^3 = U_2(x)M_0 - U_1(x)I$, where $U_n(x)$ is the nth-order Chebyshev polynomial of the second kind, and $x = \mathrm{Tr}(M_0)/2$. We now make an important observation. It can be easily checked that, if $U_2(x)$ becomes equal to *zero* for some value of energy, this choice automatically fixes $U_1(x)$ equal to ± 1. Since $U_1(x) = (E-\epsilon_0)/t$, we have a special energy $E = \epsilon_0 \pm t$ that simultaneously ensures

$U_2(x) = 0$ and $U_1(x) = \pm 1$. At this special energy the matrix M_0^3 simply becomes equal to $-I$.

Let us now consider the case $E = \epsilon_0 + t$, and look at the amplitudes of the electron wavefunction at different sites on the chain at this specific value of the electron energy. For $E = \epsilon_0 - t$ we can proceed in a similar way. Using equation (5) and the above conditions simultaneously, we see that the wavefunction amplitudes at the sixth and fifth atomic sites from the left are given by $\psi_6 = -\psi_3 - \lambda_2\psi_2$ and $\psi_5 = -\psi_2$ respectively. It is then easy to calculate the remaining amplitudes up to infinite distance in terms of the amplitudes at the second and the third sites. It is interesting to observe that hierarchy in on-site terms is introduced at sites with index $(3n+2)$, $n = 0, 1, 2, \ldots$ from the left, and that the amplitudes at each of these sites are always equal to $\pm\psi_2$. Amplitudes on the sites other than these become a linear combination of ψ_3 and ψ_2; more specifically, each of them are of the form $\pm[\psi_3 + (\sum_n c_n\epsilon_n)\psi_2]$, where c_n are integers. Now, if an eigenstate is of an extended type, then it has to be non-vanishing even at infinite distance away from the first site (extreme left), and at the same time it has to remain finite throughout the lattice. The finiteness of amplitudes at sites other than the $3n + 2$, $n = 1, 2, \ldots$), sites depends on the growth of the factor $\sum_n c_n\epsilon_n$ and it is not *a priori* possible to estimate whether it always remains finite at the desired energy $E = \epsilon_0 + t$. On the other hand, if ψ_2 can be made to vanish at this energy, then ψ_{3n+2} is always equal to zero for any integral value of n. At the same time it automatically ensures that the amplitudes on the remaining sites will be equal to $\pm\psi_3$. To understand this we consider the first few in the hierarchy of equations (2), namely

$$(E - \epsilon_L)\psi_1 = t\psi_2 \tag{6}$$

$$(E - \epsilon_1)\psi_2 = t\psi_1 + t\psi_3 \tag{7}$$

$$(E - \epsilon_0)\psi_3 = t\psi_2 + t\psi_4 \tag{8}$$

and so on. We now observe that, since expressing an amplitude on any arbitrary site in terms of sites 2 and 3 does not demand any specic value of ϵ_L, its choice remains free. We therefore choose the site energy of this edge atom to be equal to $\epsilon_L = E = \epsilon_0 + t$. From (6) it becomes obvious that this choice of ϵ_L makes ψ_2 equal to zero, and, consequently, each subsequent $\psi_{3n+2}(n = 1, 2, 3, \ldots) = 0$. The electron thus feels an effective 'periodic' arrangement of identical atoms with site energy ϵ_0 (except the one on the extreme left). Setting ψ_1 equal to unity, we can easily obtain the amplitude at the third site $\psi_3 = -1$, and at all other sites to be equal to ± 1. The wavefunction profile that spans the 1D hierarchical system in this case is typically of the form $1, 0, -1, -1, 0, 1$ for the first six sites, and this pattern is repeated periodically up to infinite distance for the particular energy $E = \epsilon_0 + t$. This is a Bloch-like extended eigenfunction for the Vicsek fractal and the above energy E is definitely an eigenvalue.

The problem now is to find out whether there are other energy eigenvalues for which the fractal sustains extended states. For this, we consider a renormalized version of the 1D hierarchical chain. We can do this by decimating the sites with site energy ϵ_0 and ϵ_L. The recursion relations for the first three sites are given by

$$\epsilon_L' = \epsilon_1 + t^2[1/(E - \epsilon_L) + 1/P] \tag{9}$$

$$\epsilon_0' = \epsilon_1 + 2t^2/P \tag{10}$$

$$t' = t^3/[P(E - \epsilon_0)] \tag{11}$$

$$\epsilon_1' = \epsilon_2 + 2t^2/P \tag{12}$$

where $P = (E - \epsilon_0) - t^2/(E - \epsilon_0)$. Similar relations can be obtained for the other on-site terms also. Renaming the surviving sites we find the lattice to have exactly the same

hierarchical distribution of modified on-site potentials as in the original lattice. Therefore, using the same set of arguments we find that the values of energy at which $\psi_{3n+2} = \pm\psi_2$ for $n = 1, 2, \ldots$ on the renormalized lattice are obtained by setting $E = \epsilon_0' + t'$. Hence, if ψ_2 on this renormalized lattice becomes zero at the above energies, then the wavefunction at all $3n + 2$ sites on that length scale will vanish. But, we have to be alert to the fact that in order to make $\psi_2 = 0$ on the renormalized lattice we must have $E = \epsilon_L'$ at those specific energies. Now, the value of ϵ_L in the original chain has already been fixed to be $\epsilon_0 + t$. So, the possibility of having $\psi_2 = 0$ on the renormalized lattice depends entirely on whether we can still achieve the equality $E = \epsilon_L'$ with the pre-determined value of the edge site energy. Exploring this aspect we find that it is quite simple to prove that, if we have the equality $\epsilon_L(n) = \epsilon_0(n) + t(n)$ at any nth stage of renormalization, then this equality holds for all subsequent iterations. That is to say, a 'proper' choice of the edge site energy at the very first stage (in the original lattice) ensures the existence of extended electron states at all subsequent length scales. The energy values corresponding to these extended states are obtained by solving the polynomial equation $E = \epsilon_0(n) + t(n)$ at the nth stage. It then becomes straightforward to trace back and calculate the amplitudes on the original fractal lattice. The wavefunction is now found to have longer periods with increasing n. However, it should be appreciated that all the energies obtained this way may not be the 'allowed' ones. The allowed energies will be those for which ϵ_i, $i = 1, 2, 3, \ldots$, will remain finite. For example, setting $\epsilon_0 = 0$ and $t = 1$, we find $E = 1$ at the beginning. At this energy the amplitudes on each site on all the upper and lower side branches are zero. The propagating electron will not feel the presence of the dangling edges of the fractal at this energy. On scaling, we obtain $E = -2$, $-0.801\,938$, $0.554\,958$ and $2.246\,98$ from the first iteration. In this case we have to check only the finiteness of ϵ_1. It remains finite at each of these energy values. Therefore these energies are allowed. The amplitudes now start developing non-zero values at some of the sites with co-ordination number four as well as at the side branches attached to these sites. The number of non-zero amplitudes will increase with the progress of renormalization. Carrying on this process we will be able to generate the full spectrum of extended eigenstates.

In conclusion, we have shown the existence of Bloch-like states on a fractal lattice. The method can be applied to other loopless fractals exploiting their self-similarity and the possibility of a disorder induced insulator–metal transition can be investigated. A complete analysis of the eigenstates and a study of electrical conductance on such systems will be reported elsewhere.

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