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Exact results for infinite and finite Sierpinski gasket fractals: extended electron states and transmission properties

Arunava Chakrabarti†

Department of Physics, University of Kalyani, Kalyani, West Bengal 741 235, India

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Abstract. We present an exact calculation to show that an infinite Sierpinski gasket fractal supports an infinite number of *extended* electron states. We work within the real space renormalization group (RSRG) scheme and show that by analysing the recursion relations for the Hamiltonian parameters one can extract the eigenvalues for an infinity of eigenstates that are of extended character. We also calculate the transmission coefficient for fractals of arbitrarily large generation. For the energy eigenvalues corresponding to the extended electron states, the transmission coefficient exhibits a novel feature. It turns out to be scale invariant with a value between zero and one depending upon the initial choice of the on-site potentials and the nearest-neighbour hopping integrals.

Fractals have been studied by condensed matter theorists for many years. One of the main points of interest has been the fact that these self-similar objects are found to serve as a non-trivial model for the backbone of a percolating cluster [1, 2]. Works with the popular Sierpinski gasket (SG) fractal have confirmed this idea [3]. Fractals, in particular the deterministic fractals (the SG is one such example), possess scale invariance (dilation symmetry) and do not have any translational order.

Statistical physics on fractal lattices constitutes a large volume in the literature (see [1–3] and references therein). However, the study of their electronic properties is not that exhaustive. As fractals exhibit the absence of translational invariance and presence of self-similarly at the same time, they may be thought to bridge the gap between periodic (ordered) and randomly disordered systems. These systems belong to a class different from that of the quasiperiodic lattices that have drawn considerable attention in recent years [4–6]. Therefore, a detailed study of the electronic properties of fractals may lead to new results and insight into the physics of non-periodic systems.

An early study of electronic properties of fractal lattices is due to Domany *et al* [7] who solved the Schrodinger equation on a variety of fractal lattices to examine the energy spectrum using a recursive technique. However, this work does not discuss the precise nature of the electronic wave functions. The energy levels have been reported to be discrete, very closely spaced, and highly degenerate [7]. Rammal and Toulouse [8] studied the energy spectrum of an SG in presence of a magnetic field. There has also been some

† E-mail address: rkm@cmp.saha.ernet.in and arunava@klyuniv.ernet.in

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work on the electronic properties of a non-branching Koch fractal based on a real space decimation method in which the scaling properties of the spectrum and the quantum states have been discussed [9]. From these studies the electronic wave functions appear, in general, to be localized, exponentially, or otherwise. Localization of wave functions on a fractal lattice is not unexpected, because of the absence of translational order. However, it should be mentioned here that the absence of translational invariance is not necessarily an obstacle in getting extended electron states in a system. Such situations arise in the cases of one-dimensional random, as well as quasiperiodic, systems, as has been reported recently [10–12]. In all the above cases, the positional correlation between a particular set of atomic sites has been shown to be responsible for the existence of extended states via a resonant tunnelling mechanism, or otherwise [12]. In fractal lattices however, such positional correlations are, in general, absent. Hence, the possibility that these lattices can support extended electronic states does not seem obvious. Therefore, we find it rather interesting to investigate such a possibility, and also to find the energy eigenvalues at which the lattice will support extended electron states, if they exist. We find an additional motivation from a recent result [13], where it has been shown analytically that a semi-infinite Vicsek fractal can support an infinite number of extended eigenstates if one *tunes* the atom at one edge properly.

In this paper we deal with the well known Sierpinski gasket fractal. Our work is divided into two parts. First, we do an RSRG study of the fractal by analysing the recursion relations of the Hamiltonian parameters. Working within a tight-binding formalism we show that the fractal lattice indeed supports an infinity of extended electronic states. Analysing the recursion relations of the Hamiltonian parameters we explicitly calculate the energy eigenvalues responsible for these extended electronic eigenstates. We also discuss which eigenvalues are to be 'discarded' as far as the extended states are concerned. Secondly, we calculate the end-to-end transmittance of finite SG lattices of arbitrarily large generations connected between two ordered leads at the two vertices. By using the transfer matrix method (TMM) [14] we show that, at all the energies for which the infinite SG lattice supports extended states, the finite versions may have any value of the transmission coefficient between zero and one if we assign a suitably chosen value of the site energy to the 'border' atoms. The transmission coefficient, for a given set of parameters, turns out to be *invariant* even if we increase the system size indefinitely. This non-zero fixed value of the transmission coefficient can be taken as a tool to characterize the different extended wave functions for the fractal system.

We start by describing an infinite SG lattice by the usual tight-binding Hamiltonian in the Wannier representation 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, which in our case are taken to be equal to ϵ and t respectively everywhere. In figure 1(a) we show a part of the infinite lattice. To examine the eigenvalues and eigenfunctions we have to solve a set of difference equations, *viz.*

$$(E - \epsilon)\psi_n = t(\psi_i + \psi_j + \psi_k + \psi_l) \tag{2}$$

for all lattice points denoted by n. i, j, k and l are the four nearest neighbours of the nth site. We now renormalize the system by eliminating a subset of the above equations in terms of the rest. A part of the renormalized lattice consisting of the undecimated sites is shown in figure 1(b). A set of recursion relations for ϵ and t is then obtained, and is given

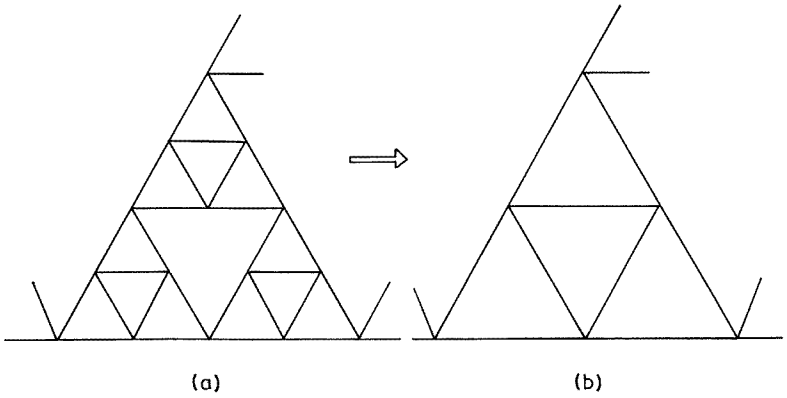

Figure 1. (a) Part of an infinite Sierpinski gasket and (b) its renormalized version.

by

$$\epsilon_{n+1} = \epsilon_n + 4t_n^2(E - \epsilon_n)/D_n \tag{3}$$

$$t_{n+1} = t_n^2(E - \epsilon_n + 2t_n)/D_n. \tag{4}$$

Here, $D_n = (E - \epsilon_n)(E - \epsilon_n - t_n) - 2t_n^2$. The subscript n refers to the nth stage of renormalization. At this point is should be mentioned that, in a recent paper, Wang [15] has reported the existence of extended electronic eigenstates on an SG lattice. Our work differs from that of [15] in the sense that we study here the evolution of the full parameter space consisting of both ϵ and t, whereas Wang has started with a special model in which ϵ is set equal to zero at the very outset, and has been forced to assume the value zero at all stages of iteration. Simply be considering the full parameter space comprising both ϵ and t, we derive results that differ from those obtained in [15]. Artificially contracting the dimension of the parameter space from two to one not only excludes energy eigenvalues that really belong to the extended states, but can lead even to *erroneous* conclusions regarding their nature, as we will see. We now proceed to describe our way of looking at the problem.

It is interesting to see from the recursion relations that if, at any stage of renormalization n, the electron energy E happens to be equal to the site energy ϵ_n at that stage, then we immediately get $\epsilon_{n+1} = \epsilon_n$ and $t_{n+2} = -t_{n+1} = t_n$ for all subsequent stages of renormalization. This implies that the hopping integral reaches a two-cycle fixed-point under renormalization for this particular value of the energy, i.e. $E = \epsilon_n$. If this fixed point of t turns out to be different from zero then looking at the fractal lattice at any stage of RSRG we find non-zero overlap of wave functions between nearest-neighbouring sites at that length scale. This conclusively proves that we have an *extended* eigenstate for the energy concerned. For example, to start with, if we select a model with the initial value of the site energy $\epsilon = 0$ and $t = 1$, then we find that for $E = 0$ the site energy reaches its fixed-point value (equal to zero) for all subsequent iterations. Under this condition we additionally get $t_1 = -t = -1$ and $t_2 = t = 1$ after the first two RSRG steps, and this goes on indefinitely. We thus have an extended electron state at $E = 0$ for the above model. The distribution of the amplitudes of the wave function for $E = 0$ is shown in figure 2(a). It is to be noted that we have not forced t beforehand to assume a non-trivial fixed-point value, but it naturally flows into a two-cycle loop once the energy is selected to be equal to the on-site potential. This idea helps us in extracting other energy values for

which one can have extended states for the same model. If, for example, we demand the equality $E = \epsilon_1$ after one-step renormalization, we find it leads to a polynomial equation in E. Solving this equation we come across values of E among which the 'allowed' values (for extended states) will be those for which the hopping integral from the second stage of iteration, i.e. from t_2 onwards, will flow naturally in a two-cycle loop with a non-zero value. We obtain $E = 0$ and $E = 3$ by solving the equation $E = \epsilon_1$ with $\epsilon = 0$ and $t = 1$. This particular result is in total disagreement with that in [15] where $E = 0$ and $E = 3$ have been erroneously declared to correspond to 'critical' states showing a power-law decay.

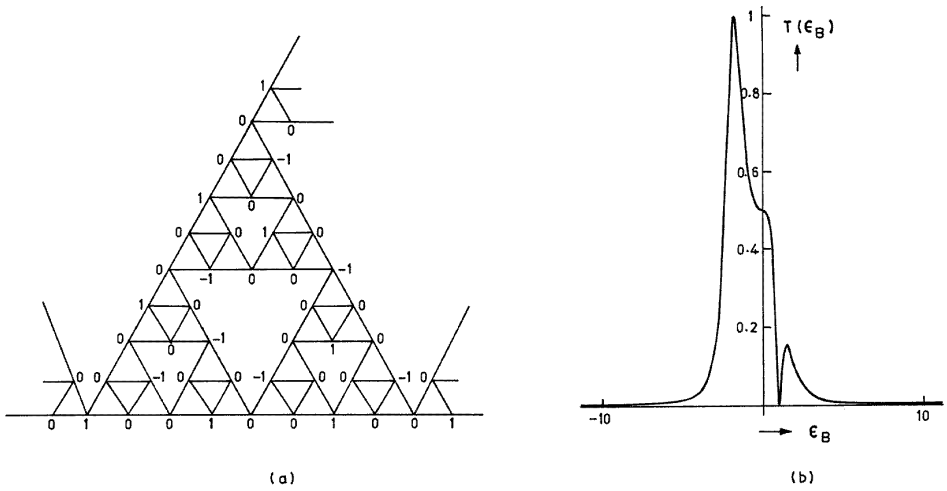

Figure 2. (a) Amplitudes of an extended wavefunction for $E = 0$ with $\epsilon = 0$ and $t = 1$; (b) variation of the transmittivity as a function of the site energy of a border atom. Here, $E = 0$, $\epsilon = 0$ and $t = 1$.

We now try to generalize the situation and discuss the conditions that have to be fulfilled in order that an energy calculated from the polynomial equation $E - \epsilon_n = 0$ gives an eigenvalue corresponding to an extended state. From the recursion relations (3) and (4) it is very simple to show that, if $E = \epsilon_n$ at any nth stage of iteration, then we have an equation

$$(E - \epsilon_{n-1})(E - \epsilon_{n-1} + 2t_{n-1})(3t_{n-1} - E + \epsilon_{n-1}) = 0. \tag{5}$$

That is, we now have to extract E from three different polynomial equations given by

$$E = \epsilon_{n-1} - 2t_{n-1} \tag{6}$$

$$E = \epsilon_{n-1} \tag{7}$$

$$E = \epsilon_{n-1} + 3t_{n-1}. \tag{8}$$

Now for all energy values that are obtained as solutions of equation (6) it can be easily checked from (4) that the hopping integral t_n in the next stage of renormalization and, consequently, at all subsequent stages flows to zero. Therefore, one cannot expect extended eigenstates to exist for these values of the energy. Solutions arising out of equation (6) are therefore *disallowed* as far as the extended eigenstates are concerned. On the other hand, solutions obtained from equation (8) keep t_n non-zero and oscillating in a two-cycle loop. It is easy to show that for these energy values $t_n = 1.25t_{n-1}$. If t_n is non-zero, then t_{n-1} also must be non-zero. In this way the recursion relation (4) connecting t_n and t_{n-1} can be made to work in the reverse direction to show that the hopping integrals at all the previous steps

should remain non-zero for $E = \epsilon_{n-1} + 3t_{n-1}$. Other allowed values of the energy will result from the equation $E = \epsilon_{n-1}$, as has already been discussed. We find it rather interesting that at each stage of renormalization the energy values corresponding to the extended states come in a typically paired manner, such that the sum of the allowed roots occurring in such a pair will always be $2\epsilon + 3t$. Thus, in the model where $\epsilon = 0$ and $t = 1$, the energy eigenvalues corresponding to extended eigenstates are found to be $E = (0, 3)$ from the first stage of renormalization, $E = (0, 3)$, and $(-0.791\,287\,847\,477\,92, 3.791\,287\,474\,7792)$ from the second level (i.e. as solutions of the equation $E = \epsilon_2$) and so on. The sum of the pairs in the brackets is clearly seen to be three (which is equal to $2\epsilon + 3t$, with $\epsilon = 0$ and $t = 1$) in all cases. This result has been checked to be true for solutions obtained from higher-order equations as well. It is therefore tempting to put this relationship between the roots of the equation $E - \epsilon_n = 0$ in the form of a *condition* which must be satisfied by values of E obtained from the above equation in order that they correspond to the extended eigenstates for the gasket. The spurious solutions of the relevant polynomial equations can thus be eliminated. As the RSRG operation can proceed indefinitely, its quite clear that one can have an infinite number of extended electronic eigenstates in a infinite SG fractal lattice.

Having analysed the case of an infinite fractal, we now turn our attention to a finite SG lattice. In particular, we focus on the possibility of having a non-zero end-to-end transmission of a wave packet incident on a finite SG fractal or arbitrarily large size through a pair of leads connected to the two vertices at the base of the triangle enclosing the entire structure. The site energies of the boundary atom will affect the transmission. In what follows, we, instead of making a scan over the entire spectrum of eigenvalues (known to be a Cantor set [7]), choose only those energies which have been shown in this article to give rise to extended electronic eigenstates for the infinite fractal. By doing this we can make a classification between the different extended wave functions based on their transmission properties. We assign a site energy ϵ_B to each of the three boundary sites. Then after n-step renormalization, a lattice comprising of $3 + 3(3^n - 1)/2$ sites (including the three outermost atoms) can be transformed into a cluster of three sites which formed the boundary of the original lattice, but now with modified site energies and the nearest-neighbour hopping integral. From this three-site cluster we generate a pair of sites each with a site energy $\tilde{\epsilon_B} = \epsilon_B(n) + t_n^2/[E - \epsilon_B(n)]$, and an effective hopping integral connecting the above pair, *viz.*, $\tilde{t} = t_n + t_n^2/[E - \epsilon_B(n)]$. The value of the site energy of the border atom at any stage n is given by $\epsilon_B(n)$, and is related to its value at an earlier stage by the equation

$$\epsilon_B(n) = \epsilon_B(n-1) + 2t_{n-1}^2(E - \epsilon_{n-1})/[(E - \epsilon_{n-1})(E - \epsilon_{n-1} - t_{n-1}) - 2t_{n-1}^2]. \tag{9}$$

It is immediately seen that, whenever E is chosen to be equal to ϵ_{n-1}, ϵ_B also flows to the fixed point, i.e. $\epsilon_B(n) = \epsilon_B(n-1)$ for all subsequent values of n.

An ordered lead of identical atoms of site energy ϵ_0 (set equal to zero) and hopping integral t_0 is attached to the two border atoms of the SG at the two ends. The problem now reduces to that of studying the transmission through a 'dimer impurity' placed in an otherwise periodic infinite chain. The transfer matrix M [14] across the pair of impurity sites then has the matrix elements

$$M_{11} = (E - \tilde{\epsilon_B})^2/t_0\tilde{t} - \tilde{t}/t_0 \tag{10}$$

$$M_{12} = -(E - \tilde{\epsilon_B})/\tilde{t} \tag{11}$$

$$M_{21} = -M_{12} \tag{12}$$

$$M_{22} = -t_0/\tilde{t}. \tag{13}$$

It is now easy to see that if there exists an energy E that simultaneously makes $\tilde{t} = t_0$ and $E = \tilde{\epsilon_B}$, then at this particular energy the 'defect' transfer matrix will offer identity contribution (with a negative sign) and one should have full end-to-end transmission across the entire lattice. To explicitly see whether such a possibility exists, we consider the model in which $\epsilon = 0$ and $t = 1$. At $E = 0$ the infinite lattice has already been shown to possess an extended eigenstate in this model. Let us now work with a finite-sized gasket at an even generation, say, $2n$. Then with the above choice of E, it immediately turns out that $\epsilon_{2n} - \epsilon$, $\epsilon_B(2n) = \epsilon_B$, and $t_{2n} = t$. It is now quite straightforward to calculate the transmittivity T as a function of the site energy ϵ_B of the border atom. The result is

$$T(\epsilon_B) = 4/[4(\epsilon_B + 1)^2 + ((\epsilon_B - 1)(\epsilon_B + 2) - \epsilon_B/(\epsilon_B - 1))^2]. \tag{14}$$

A plot of $T(\epsilon_B)$ against ϵ_B is shown in Figure 2(b). It is readily seen that by tuning the value of ϵ_B one can get, for $E = 0$, all possible values of the transmittivity ranging from zero to one. T in the above equation turns out to be unity if we choose, in this model, $\epsilon_B = -1.769\,29$. With this set of the Hamiltonian parameters one can seek the value of the transmission coefficient for all the energies corresponding to the extended electronic states. T is no longer unity for these other energy values (different from $E = 0$), but remains invariant with increasing system size. The constant value of T depends on whether we are calculating it for an 'even'- or an 'odd'-numbered generation. The invariance of T becomes apparent when one realizes that for all such extended state eigenvalues the site energies ϵ and ϵ_B, and the nearest-neighbour hopping integral t, get locked in their fixed-point values, thereby rendering the transfer matrix elements M_{ij} scale invariant. However, the generation after which the scale invariance of T sets in, depends on the choice of the RSRG iteration number n for which we set $E = \epsilon_n$. Thus, with $E = 0$, $\epsilon = 0$ and $t = 1$ with ϵ_B arbitrarily chosen, T will be a constant from the very first stage of the renormalization process, whereas, for $E = 3$, say, the invariance of T sets in from the second stage, and so on. The fact that T becomes independent of the system size N is to be contrasted, for example, with the 1D quasiperiodic copper mean chain where the matrix M across a 'dimer' [11] becomes identity for all energies corresponding to the extended states, making the quasiperiodic chain at those energies equivalent to a perfectly ordered chain of atoms, or with the case of a loop-less Vicsek fractal where one finds a power-law decay for T even for extended electronic states in the thermodynamic limit [16].

In conclusion, we have been able to evaluate eigenvalues for a set of extended electronic states in an infinite Sierpinski gasket. The transmission coefficient for arbitrarily large finite gaskets show the novel feature of being invariant with increasing system size.

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