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Sierpinski gasket in a magnetic field: Electron states and transmission characteristics

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The Sierpinski gasket fractal has been studied in the presence of a magnetic field applied perpendicular to the plane of the fractal. The discretized Schrödinger equation for a single electron is solved using an exact real-space decimation technique. An infinite number of energy eigenvalues exist that give rise to perfectly extended eigenstates on this fractal. A prescription for their evaluation is proposed. Aharonov-Bohm oscillations in the transmission coefficient have been investigated in the case of this fractal lattice. The nature of oscillations for different electron energies and its dependence on the system size as well as on the boundary sites are discussed in detail. [S0163-1829(97)02745-8]

The electronic and other physical properties of regular fractal lattices have been quite popular subjects of study in condensed matter and statistical physics for many years.[1–6] A very well-studied model has been the Sierpinski gasket (SG). In 1982, Domany *et al.*[1] solved the Schrödinger equation for a single tightly bound electron on a SG using a real-space decimation scheme. The energy levels are found to be discrete, very closely spaced, and highly degenerate. These gaskets have the interesting property that they are self-similar under a scale transformation and have a hierarchy of loops. This structure leads to a Cantor set energy spectrum and to the localization of almost all the one-electron states as has been observed in Ref. 1. This localization is structure induced and not disorder induced as in the case of Anderson localization. Rammal and Toulouse[7] extended the earlier work on the SG to include a magnetic field given perpendicular to the plane of the gasket. Such a field, as was shown in a later publication by Banavar *et al.*,[8] changes the qualitative feature of the energy spectrum. A majority of the eigenfunctions become extended in character. However, a precise determination of these eigenfunctions or the corresponding eigenvalues could not be made. Their conclusions were based on a numerically done ''escape rate'' counting and studying the inverse participation ratio at energies obtained by diagonalizing a lattice of a finite number of sites.

Very recently, interest in the electronic spectrum of some regular fractal lattices has been renewed. Exact results have been obtained based on renormalization-group methods which show that some regular fractals like the SG and the loopless Vicsek fractal are capable of sustaining an infinite number of extended eigenstates.[9–12] These extended states exhibit different behaviors depending on the lattice geometry. Such behaviors may be reflected in, say, the end-to-end transmission coefficient for arbitrarily large finite fractal lattices.[11,12] Precise rules for evaluating the eigenvalues corresponding to these extended eigenstates have been prescribed based on an analysis of the recursion relations of the parameters of the Hamiltonian under the renormalization-group transformation.[12,13]

In this paper we discuss the case of a Sierpinski gasket fractal in a magnetic field applied perpendicular to the plane of the fractal. We use a real-space renormalization-group (RSRG) scheme. Our interest is twofold. First, we wish to reexamine the effect of a magnetic field on the energy spectrum of the infinite gasket. In particular, we calculate the eigenvalues that will correspond to the extended states in the presence of a magnetic field. Second, we investigate the Aharonov-Bohm oscillations in the transmission coefficient for arbitrarily large fractal lattices in the presence of a magnetic field. A magnetic field is already known to produce such oscillations in the conductance (or transmittance) in various physical systems.[15–17] Even in the case of a simple tight-binding ring of atoms one gets interesting observations regarding the periodic behavior of the conductance, as well as its dependence on different physical parameters.[18] However, a study of oscillations of the transmittance for fractal lattices is still lacking. As a Sierpinski gasket possesses loops at all scales of length, the behavior of the transmission coefficient as a function of the magnetic field, to our mind, is going to be a highly interesting study. We propose to investigate in detail the dependence of the period of oscillations on the size of the lattice along with the effect of boundary sites on the transmittance and its period for this particular fractal.

Our results are quite interesting. We find that at $E=\epsilon$, where ϵ is the site energy of the fractal lattice and E is the energy of the electron, we have an extended eigenstate. This value of E is found to be independent of the field strength. Other energies corresponding to the extended states depend on the strength of magnetic field.

As far as the transmittance of finite lattices is concerned, we find that the transmission coefficient exhibits periodic oscillations with respect to the applied field. Results have been obtained for energies that correspond to the extended eigenstates for the infinite fractal. The role of edge atoms in a finite lattice has been observed to be rather interesting as will be discussed later on. The general trend is that the lattice in the presence of the field exhibits a larger transmission than in the absence of the field, which is in agreement with the

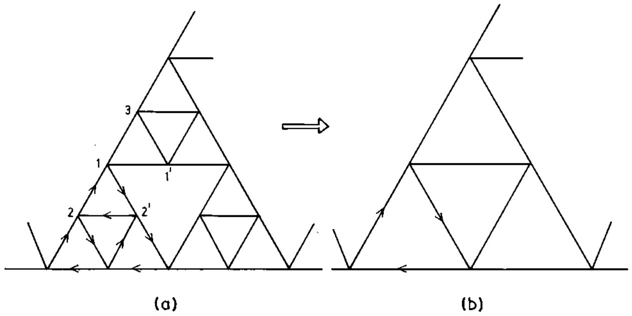

FIG. 1. (a) Part of an infinite Sierpinski gasket and (b) its renormalized version. Arrows indicating t_f or t_b have been shown in a small plaquette only.

results of Banavar *et al.*[8] that a whole lot of eigenstates now possess an extended character. In what follows, we develop our ideas and give the results in details.

We start by describing a single electron on an infinite SG lattice by the usual tight-binding Hamiltonian in the Wannier representation in presence of a magnetic field:[19]

$$H=\sum_i \epsilon|i\rangle\langle i|+\sum_{\langle ij\rangle}[t_f|i\rangle\langle j|+t_b|j\rangle\langle i|], \qquad (1)$$

where ϵ is the on-site potential at all the atomic sites. $t_f=te^{i\gamma}$ and $t_b=te^{-i\gamma}$ are the ''forward'' and ''backward'' hopping integrals, respectively. Throughout the discussion we will take $t=1$. The effect of the magnetic field is to introduce a phase in the nearest-neighbor hopping integral.[19] We have defined $\gamma=2\pi\phi/\phi_0$, where ϕ_0 is the flux quantum hc/e.

In Fig. 1(a) we show a part of the infinite lattice. Following Banavar *et al.*[8] we select a flux distribution in which all bonds in the direction of the arrows have the nearest-neighbor hopping matrix element t_f and all bonds opposite to the arrows have a matrix element t_b. All the elementary upward-pointing triangles have the same flux 3ϕ, while for the smallest downward-pointing triangle it is -3ϕ. To examine the eigenvalues and eigenfunctions we have to solve a set of difference equations. A typical equation looks like

$$(E-\epsilon)\psi_1=t_f(\psi_{2'}+\psi_3)+t_b(\psi_2+\psi_{1'}). \qquad (2)$$

In Eq. (2) ψ_i represents the Wannier orbital at the ith site and the subscripts denote site indices as shown in Fig. 1(a). Other equations can be formed in a similar fashion. Here, $t_f=te^{i\gamma}$, and t_b is its complex conjugate. The site energy is taken to be the same and equal to ϵ at all sites. We decimate all the sites appearing on the right-hand side of Eq. (2). Sites similar to site 1 are kept undecimated as can be identified by comparing Figs. 1(a) and 1(b). A part of the renormalized lattice consisting of the undecimated sites is shown in Fig. 1(b). Recursion relations for the on-site terms and the hopping integrals are then obtained, and are given by

$$\epsilon_{n+1}=\epsilon_n+2[A_n t_f(n)+B_n t_b(n)]/D_n, \qquad (3)$$

$$t_f(n+1)=[t_f(n)B_n+t_b(n)C_n]/D_n, \qquad (4)$$

$$t_b(n+1)=t_f^*(n+1). \qquad (5)$$

Here,

$$A_n=[(E-\epsilon_n)t_b(n)+t_f(n)^2], \qquad (6)$$

$$B_n=[(E-\epsilon_n)t_f(n)+t_b(n)^2], \qquad (7)$$

$$C_n=2t_f(n)t_b(n)+[t_f(n)^3+t_b(n)^3]/(E-\epsilon_n), \qquad (8)$$

$$D_n=(E-\epsilon_n)^2-3t_f(n)t_b(n)-[t_f(n)^3+t_b(n)^3]/(E-\epsilon_n). \qquad (9)$$

Here, n in the subscript or in the parentheses refers to the nth stage of renormalization.

From the recursion relations listed above, it is not difficult to find out that if we choose $E=\epsilon_n$ at any stage n, then for all subsequent stages of renormalization we have $\epsilon_{n+1}=\epsilon_n$ and $t_f(n+2)=-t_f(n+1)=t_f(n)$. An identical behavior for t_b naturally follows. This implies that we get a two-cycle fixed point for the hopping integrals. To be specific, if we select $E=\epsilon$ at the very beginning, then for all subsequent stages of renormalization the parameters get locked in their respective fixed point values with the hopping integrals fixed at nonzero values. This indicates that we have an extended eigenstate at $E=\epsilon$.[12] This idea can be carried onto any stage of renormalization and by equating E to ϵ_n at that stage we can extract an infinity of extended electron eigenstates, if n is infinitely large. However, a few points are worth discussing here. First of all, it is interesting to observe that the eigenvalue $E=\epsilon$ obtained at the initial level is independent of the strength of the magnetic flux threading the fractal space. Incidentally, the same energy value also corresponded to an extended state in the absence of field.[12] However, the energy values obtained from progressively higher stages of the RG are dependent on the flux. Second, from the recursion relations it is very simple to show that, if $E=\epsilon_n$ at any nth stage of iteration, then we have an equation

$$(E-\epsilon_{n-1})\{(E-\epsilon_{n-1})^3-7t_f(n-1)t_b(n-1)-3[t_f(n-1)^3+t_b(n-1)^3]\}=0. \qquad (10)$$

It is seen from the above equation that all the roots that were the solutions of the equation $E-\epsilon_{n-1}=0$ are also the solutions at the next level. The other roots may be obtained from the solution of the equation $(E-\epsilon_{n-1})^3-7t_f(n-1)t_b(n-1)-3[t_f(n-1)^3+t_b(n-1)^3]=0$. However, not all of them are allowed solutions. It can be shown that the energy values for which the quantity D_n in the recursion relation (4) becomes zero are disallowed solutions as far as the extended states are concerned. Also, there may not even be a state at that particular energy. The latter statement can be verified by taking a look at the density of states. We take a specific example. Let us solve the equation $E=\epsilon_n=0$ for $n=1$ and 2 with $\gamma=\pi/2$. We get the solutions $E=0, \pm\sqrt{7}$ from the first level, and $E=0, \pm\sqrt{7}, \pm 3.298\,930\,859, \pm\sqrt{3}, \pm 2.363\,836\,68$, and $\pm 1.236\,661\,365\,825$ from the second level. We find that the roots are symmetric around the value $E=0$ and that all of them correspond to the extended eigenstates. This last result can be easily verified by looking at the flow of the hopping integrals under successive renormalization steps. We have also calculated the local density of states for the infinite gasket for different values of the magnetic flux and present the result for $\gamma=0$ and for $\gamma=\pi/2$ only in Fig. 2. We find that the density of states (DOS) is perfectly

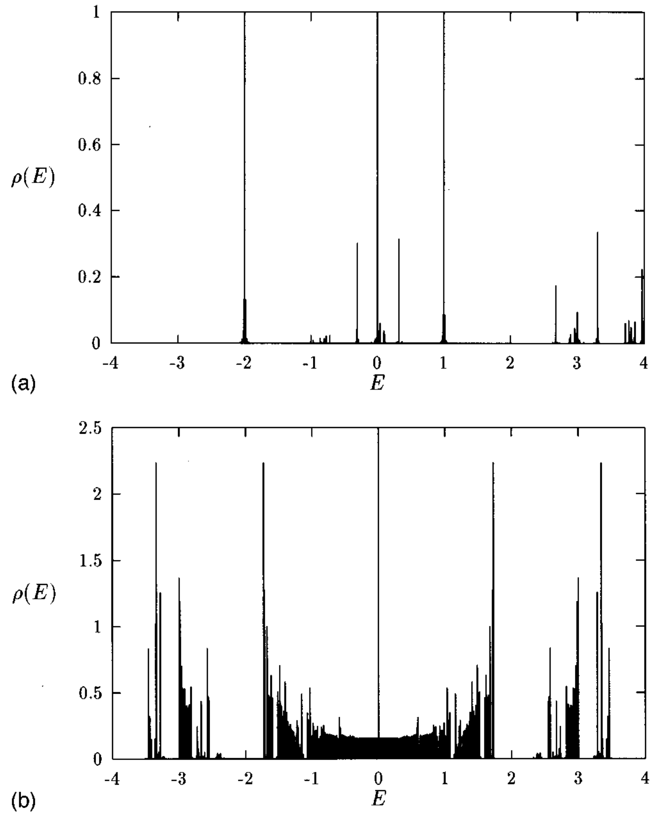

FIG. 2. (a) (Local) density of states for an infinite gasket in absence of a magnetic field. $\epsilon=0$ and $t=1$. It should be noted that the DOS for $E=-2$ and $E=1$ have been truncated down to unity for convenience. (b) (Local) density of states in presence of a magnetic field applied perpendicular to the plane of the diagram. Here, $\epsilon=0$, $t=1$, and $\gamma=\pi/2$.

symmetric around $E=0$ for this specific γ. An interesting feature of the DOS spectrum is the almost continuous region around $E=0$. It is to be noted that in the zero-field case we do not come across such quasicontinuous parts symmetrically distributed in the spectrum around $E=0$. We have scanned the region around $E=0$ very closely. All the energy values that we have scanned through keep the hopping integrals oscillating in absolutely chaotic fashion for an indefinite number of iterations. This behavior of the hopping integrals also signals the presence of extended eigenstates at those energies. The continuous character of the DOS spectrum around $E=0$ is maintained even on a finer scan as far as we have observed. Thus we see that there can be two different types of extended electronic states in the presence of a magnetic field. For one class the Hamiltonian parameters show fixed-point behaviors, while, for the other, they, in particular the hopping integrals, oscillate chaotically without going to zero. Whether these behaviors are reflected in the tranmission characteristics or not is discussed below. We would like to point out that the features we observe in the DOS remain unaltered if we choose ϵ to be different from zero. We have also calculated the DOS for different values of the flux. For $\gamma=\pi/4$, $\pi/6$, and $\pi/8$, for example, we find the presence of locally continuous distributions in the DOS. The continuous nature persists on a finer and finer scan in the values of energy. All these observations strongly indicate the presence of a band of extended eigenstates, although we cannot give an analytical proof at this moment.

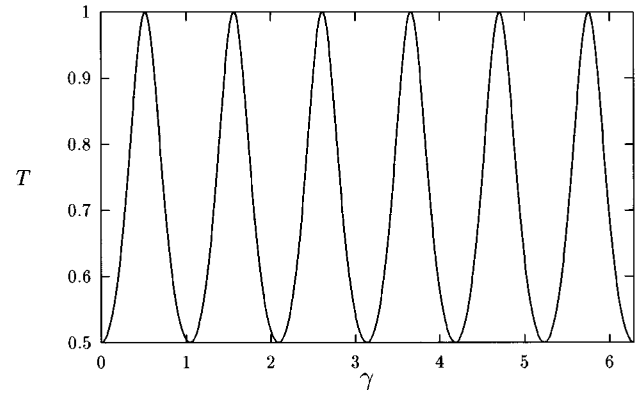

FIG. 3. Variation of the transmission coefficient (T) with the magnetic flux (γ). Here, $E=0$, $\epsilon=0$, and $t=1$.

We now concentrate on the latter part of our investigation, i.e., variation of the transmission coefficient across gaskets of arbitrarily large sizes as a function of the applied magnetic field as well as the fractal generation. To do this, we assign a site energy ϵ_B to each of the three boundary sites. Then after n-step renormalization, a lattice comprising of $3(3^n+1)/2$ 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-neighbor hopping integral. From this three-site cluster we generate a pair of sites each with a site energy $\widetilde{\epsilon_B}$ and a forward-hopping integral $\widetilde{t_f}$ connecting them. The site energy and the hopping terms are given by

$$\widetilde{\epsilon_B}=\epsilon_B(n)+t_f(n)t_b(n)/[E-\epsilon_B(n)], \tag{11}$$

$$\widetilde{t_b}=t_b(n)+t_f(n)^2/[E-\epsilon_B(n)]. \tag{12}$$

The ''backward'' hopping is, as always, the complex conjugate of the forward one. 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

$$\epsilon_B(n)=\epsilon_B(n-1)+[A_{n-1}t_f(n-1)+B_{n-1}t_b(n-1)]/D_{n-1}. \tag{13}$$

From the expressions of A_n and B_n it is seen that, whenever E is chosen to be equal to ϵ_n, ϵ_B also flows to the fixed point, i.e., $\epsilon_B(n+1)=\epsilon_B(n)$ 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 (set equal to unity) 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 P (Ref. 14) across the pair of impurity sites then has the matrix elements

$$P_{11}=(E-\widetilde{\epsilon_B})^2/\widetilde{t_f}-\widetilde{t_b}, \tag{14}$$

$$P_{12}=-(E-\widetilde{\epsilon_B})/\widetilde{t_f}, \tag{15}$$

$$P_{21}=-P_{12}, \tag{16}$$

$$P_{22}=-1/\widetilde{t_f}. \tag{17}$$

The transmission coefficient can then be calculated to be

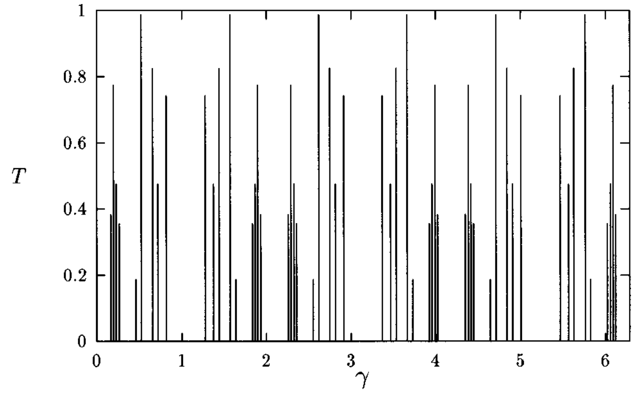

FIG. 4. Variation of the transmission coefficient (T) against the magnetic flux (γ). $\epsilon=0$, $t=1$, and $E=\sqrt{7}$ which correspond to an extended eigenstate. The hopping integrals exhibit a two-cycle fixed point. The site energies of the ''lead atoms'' have been chosen to be unity.

$$T=4\sin^2 k/[|P_{12}-P_{21}+(P_{11}-P_{22})\cos k|^2 + |P_{11}+P_{22}|^2\sin^2 k], \tag{18}$$

where k is the incident wave vector of the wave traveling through the ordered lead. We now discuss the results of the investigation on T separately.

(i) *Enhancement of T in presence of the field*. This is, of course, not unexpected if we recall our earlier discussions and, in particular refer to Banavar *et al.*[8] However, an explicit calculation can be done to visualize the effect. We do this for $E=0$ with $\epsilon=0$ and $|t_f|=|t_b|=1$. In this case a simple algebra shows that, for $\epsilon_B=0$, the transmittivity is given by

$$T=1/[1+\cos^2(3\gamma_n)], \tag{19}$$

where γ_n is the renormalized flux at the nth stage. In the absence of a magnetic field the above choice of parameters led to the value of $T=0.5$.[12] It is clear that in the presence of the field the transmittivity lies in the range 0.5–1 (see Fig. 3). Thus there is an enhancement. That this is true for the other energies as well can be checked numerically.

(ii) *Aharonov-Bohm effect in fractal space.* This is the most interesting situation which shows Aharonov-Bohm-type oscillations in the case of a fractal lattice. The results

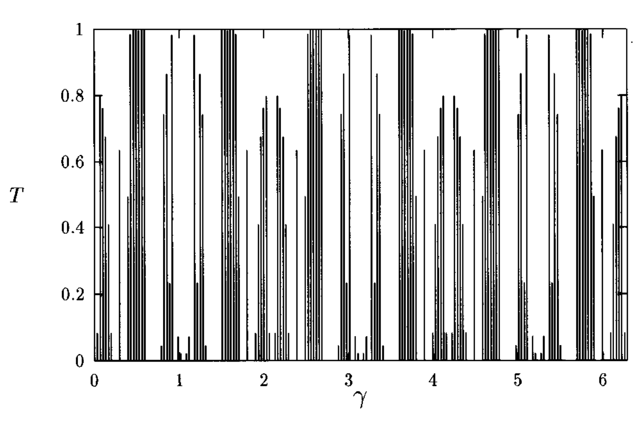

FIG. 5. T vs γ with the same parameters as in Fig. 4, except that here $E=0.3$, for which the hopping integrals oscillate chaotically. The site energies of the ''lead atoms'' have been taken as zero.

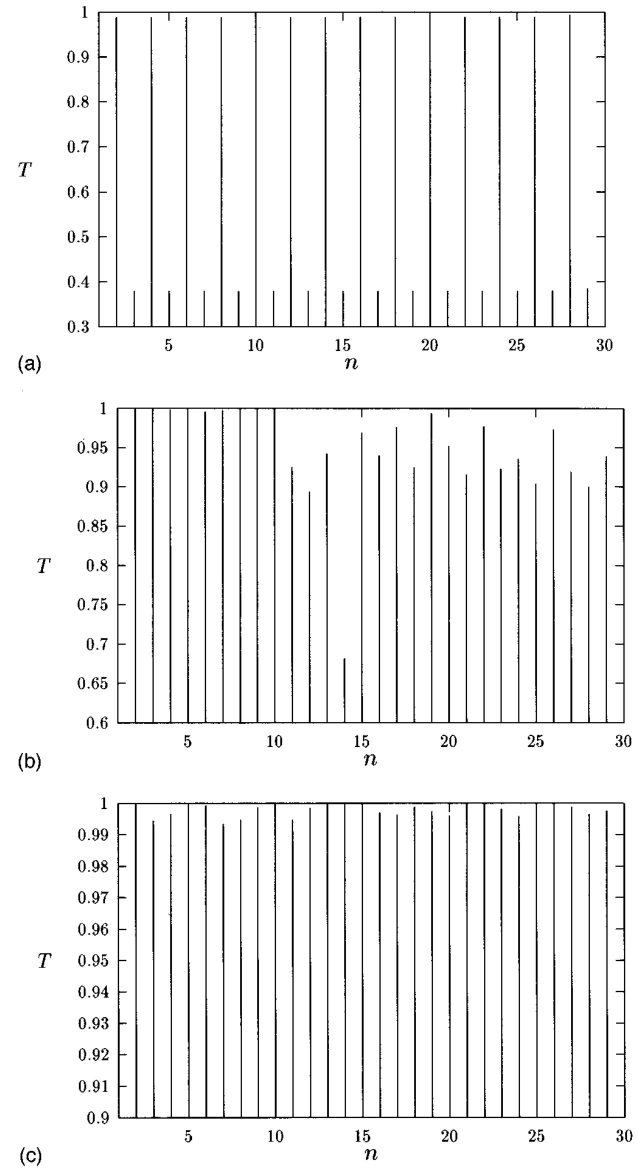

FIG. 6. Transmission coefficient (T) against generation (n). (a) $E=\sqrt{7}$, for which we have a two-cycle behavior of the hopping integrals. (b) $E=0.3$, (c) $E=0.5$. For (b) and (c) hopping integrals oscillate chaotically. In every case we have selected $\epsilon=0$ and $t=1$.

show two distinct types of variation corresponding to the ''extended state'' energies obtained from different stages of renormalization. First, we observe that with the Hamiltonian parameters chosen as in the case (i) above, for $E=0$, T oscillates following Eq. (19) above. The oscillation is periodic and the period is $\phi_0/6$ (see Fig. 3), ϕ_0 being the fundamental flux quantum. Both the period and the value of T at any field are independent of the generation of the fractal. This fact can be understood quite easily when we observe that the variation of T against γ as given by Eq. (19) above is exactly the same as that of an elementary triangular loop comprised of three atoms at the three vertices, each with site energy $\epsilon=0$ and connected by hopping integrals of absolute value unity. As a result of setting $E=0$ all the on-site energies and the hopping integrals (their absolute values) get locked in their fixed-point values which are 0 and 1, respectively, from the very first stage of the RSRG. Therefore, starting with an arbitrarily large generation fractal we bring it down, on repeated decimation of sites, to the elementary triangle talked about. The entire SG then can not be distinguished from a renormalization-group point of view, from a simple triangular plaquette having the same site energies and the hopping integrals. So at this particular energy the plane wave that is incident on the target lattice through the ordered lead fails to recognize the intricate fractal structure. The quantum interference inside the bulk destroys the information regarding the lattice topology, and the result of an elementary triangular plaquette is reproduced.

We have studied the variation of the transmittivity as a function of the applied field for the other energy values which correspond to the extended eigenstates for the infinite fractal at the same value of γ and which are obtained from the latter stages of renormalization. For all such energy values the transmittivity exhibits periodic oscillations in ϕ with a period equal to $\phi_0/3$. This period is independent of the generation number for large generations. With increasing size the transmittivity becomes fragmented but the periodic nature remains unaltered. In Figs. 4 and 5 we show the variation of T. In Fig. 4 we show the variation of T against γ for $E=\sqrt{7}$. This energy corresponds to an extended eigenstate for the infinite fractal, and has been obtained as a result of setting $E=\epsilon_2$ for $\gamma=\pi/2$. The hopping integrals exhibit two-cycle behavior. It should, however, be noted that, in order to calculate T at this particular energy, one has to suitably tune the site energy of the lead atoms so that the chosen energy falls inside the ''allowed'' band of the ''lead'' chain. The magnitude of the site energy of the lead atoms otherwise has no effect on T. In Fig. 5 we have chosen $E=0.3$. At this energy the magnitude of the hopping integrals oscillates chaotically with nonzero values for an indefinite number of iterations. This energy corresponds to an extended eigenstate of the infinite lattice, but is of a different character in the sense that the fixed-point behaviors of the Hamiltonian parameters are not observed in this case.

(iii) *Effect of the boundary site.* It is straightforward to calculate the transmittivity T as a function of the site energy ϵ_B of the border atom. The result for $E=0$ is

$$T(\epsilon_B)=4[\epsilon_B^2-2\epsilon_B\cos(3\gamma)+1]/\{4(\epsilon_B^2-1)^2+[\epsilon_B^3-2\epsilon_B+2\cos(3\gamma)]^2\}. \tag{20}$$

It is interesting to find that for values of ϵ_B other than zero, the periodicity in the variation of T against γ gets doubled. That is, while for $\epsilon_B=0$ the period is $\phi_0/6$, for nonzero values of ϵ_B it is $\phi_0/3$. It can be tested numerically that, for all values of ϵ_B other than zero and any energy E not equal to zero that corresponds to an extended eigenstate, the period of oscillation of T is completely independent of the choice of ϵ_B and is equal to $\phi_0/3$.

In addition to the above we have also investigated the variation of the transmittivity at a particular energy and field with the generation (size) of the fractal. We show our results in Figs. 6(a)–6(c). The energy values chosen are, as before, those which give rise to extended electronic states in the infinite lattice. We observe two distinct types in these graphs. The energies which correspond to the two-cycle fixed-point values of the site energies and the hopping integrals also give rise to a two-cycle periodic variation of T with the generation number [Fig. 6(a)]. If, say, the energies are obtained by solving the equation $E=\epsilon_n$, then the transmission coefficient starts exhibiting its two-cycle behavior from the $(n+1)$th generation onwards. On the other hand, if T is calculated at an energy for which the absolute values of the hopping integrals oscillate chaotically with the progress of renormalization, the transmission coefficient also fluctuates. The nature of the fluctuation can be seen in Figs. 6(b) and 6(c).

In conclusion, we have made an analytical effort to unravel the extended eigenstates that occur in a Sierpinski gasket fractal in the presence of a magnetic field applied perpendicular to the plane of the gasket. The energy $E=0$ (with $\epsilon=0$) is shown to lead to an extended state irrespective of the value of the magnetic field, whereas the other energies are field dependent. An interesting feature is the presence of a dense set of extended eigenvalues placed symmetrically around $E=0$ with $\gamma=\pi/2$. On the basis of similar observations for other values of the flux as well, we find it tempting to conjecture the presence of a ''band'' of extended states induced by the magnetic field. No analytical proof could be given, but detailed numerical tests tend to support this view for this specific value of the flux. The energy eigenvalues that have been obtained using the RSRG method are then used to study the variation of the transmittivity across arbitrarily large finite lattices. The Aharonov-Bohm-like oscillations in the transmission coefficient in the presence of the field exhibit interesting features. The periods of oscillation are different depending on whether the extended state eigenvalue is extracted at the very basic level of the system or its renormalized version. However, the periods turn out to be insensitive to the size of the lattice. The role of the boundary site for a finite gasket has also been investigated.

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