Electron states and magneto-transport in a graphene geometry with a fractal distribution of holes

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Abstract

We consider an infinite graphene geometry where bonds and sites have been removed selectively to map it onto an effective Sierpinski gasket comprising of hexagons. We show that such a structure is capable of sustaining an infinite number of extended single particle states inspite of the absence of any translational order. When each basic hexagonal plaquette in the Sierpinski geometry is threaded by a magnetic flux, the spectrum exhibits bands of extended eigenstates. The bands persist for any arbitrary value of the flux but disappear again as the flux becomes equal to half the fundamental flux quantum. The localization - de-localization issues are discussed thoroughly along with the computation of two terminal magneto-transport of finite versions of the lattice. The numerical results corroborate our analytical findings.

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1. Introduction

Graphene systems have been at the center stage of research in low dimensional systems, in particular, nano-structures, in the last decade. Both graphene systems in 2D and graphene nano ribbons have been proposed as potential candidates for various applications in nanotechnology [1] - [7]. A wide variety of problems have been investigated not only from the angle of applications, but also from the standpoint of the novel physics offered by such systems. Electronic and magnetic properties of triangular graphene rings [8], structural, mechanical and electrical properties of defect-patterned graphene nano-meshes [9], molecular transistors connected to graphene nano-ribbon electrodes [10] are among some of the recent exciting studies in the graphene system.

In recent years, several interesting experiments and theoretical works have been reported which deal with vacancies in a graphene sheet or nanoribbon. Such vacancies are usually created by ion bombardment, and in principle, the locations can be controlled almost at will. Pereira and Schulz [11] have studied the effects of vacancies on the electronic properties of a graphene sheet in the presence of a perpendicular magnetic field. The effect of an extended linear defect on the electronic transport properties of a graphene sheet has been investigated by Bahamon, Pereira and Schulz [12]. It is shown that such defects profoundly modify the properties of a nano-ribbon and even introduce new conductance quantization values. Using a first principles method Jippo, Ohfuchi and Kaneta [13] report the transport properties of graphene sheets having two- and one-dimensional periodic nano holes.

Vacancies in graphene lattice are shown to give rise to extra localized states between Landau levels [11]. The distance between the vacancies and their pattern of distribution have non-trivial effect on the physical properties of a 2D graphene geometry. The modification of the bands, the nature of the wave functions in the presence of the vacancies are inspiring in introducing such vacancies on purpose following a tailor made design [11], and look for any unusual properties that might suggest new applications.

It is thus intriguing to know what happens to the electronic states of a graphene sheet when one generates holes of increasing size, and distributes them over an infinite two dimensional graphene sheet following a pre-determined geometry. This is the central motivation behind the
present work. We undertake a detailed investigation of the single particle states on an infinite graphene sheet where holes with increasing sizes have been distributed following a Sierpinski fractal geometry [14] - [16].

Such a study serves a dual purpose. Sierpinski gasket (SPG) fractals have been well known candidates for studying percolation clusters. These self similar lattices are known to give rise to exotic electronic energy spectrum, revealing a fragmented Cantor set character [14] - [16], that has been shown later to contain an infinite number of extended eigenstates embedded in it [17] - [20]. Recently, a hexagonal Sierpinski structure has been experimentally synthesized [21]. The graphene with a Sierpinski distribution of holes lies very close to the synthesized structure, and gives us an opportunity to analyze the character of electronic states in these systems. Secondly, the present day lithographic techniques allows us to fabricate networks following any desired geometry. The potential of a graphene-fractal in the field of nano devices is thus worth investigating.

We work within a single band tight binding formalism. Several works within the tight binding formalism and with spinless, non-interacting electrons have been successful in highlighting the physical properties of graphene systems with or without defects [11] - [13]. We use the same, together with the real space renormalization (RSRG) group decimation scheme that exploits the self-similarity of a fractal geometry, to unravel the character of single particle eigenstates. The influence of a magnetic flux piercing a selected subset of the graphene hexagons on its electronic properties, is studied in details. In addition to this, the two terminal electronic transport across finite but arbitrarily large graphene-fractals is worked out.

Our results are interesting. We find that in the absence of any magnetic field, the graphene-fractal gives rise to an infinite number of extended eigenstates which coexist with the fragmented spectrum of localized states. The energies of the extended states can be precisely determined from the RSRG recursion relations. As soon as a magnetic field is switched ‘on’ in an elementary hexagon of the graphene-fractal, the density of states exhibits continuous distribution of extended states in the spectrum. These bands of extended states persist for all non-zero values of the magnetic flux $\Phi$, except for $\Phi = \Phi_0/2$, where $\Phi_0 = \hbar c/e$ is the flux quantum. At $\Phi = \Phi_0/2$ the spectrum swings back to the flux free shape with sharply localized eigenstates.
dominating the entire spectrum. Incidentally, appearance of such bands of extended states has been suggested earlier, based on extensive numerical studies by Chakrabarti [19] and Schwalm & Moritz [22] in the context of a 3-simplex fractal and a modified rectangle lattice respectively. These are self-similar lattices without any translational invariance. The existence of flux driven bands of extended states is thus curious. With the results presented in this communication we have a strong case where we can conjecture that bands of extended states might be a generic feature of deterministic fractals with holes.

In what follows, we describe the results of our calculation. Section 2 describes the model and the method. In section 3 we extract and analyze the extended eigenstates, discuss the density of states with and without the magnetic flux threading the basic plaquettes and, present the detailed results of the magneto-transport calculations for finite graphene-fractals. In section 4 we draw the conclusions.

2. The model and the method

Let us refer to Fig. 1. A selective removal of sites from the two dimensional graphene sheet will lead to a set of extended defects (voids) which distribute themselves on an effective Sierpinski fractal network [14]. With both the A (black) and B (red) sites now present in the lattice, the two dimensional geometry in fact resembles a Zachariassen fractal glass [23]. The fluctuating environment around each site generates unusual eigenstates and strange transport properties as studied earlier [17] - [20]. We shall be concerned with the effect of the parent graphene geometry on the electronic states of such a system with multiple holes. To test the effect of a magnetic flux on the spectral properties within a minimal model, we include a uniform magnetic flux $\Phi$ through each of the hexagons in Fig. 1. The system is described by the standard tight binding Hamiltonian,

$$H = \sum_i \epsilon_i |i\rangle \langle i| + \sum_{\langle ij \rangle} \left[ t_{ij} e^{i\theta_{ij}} |i\rangle \langle j| + t_{ji} e^{-i\theta_{ij}} |j\rangle \langle i| \right]$$ (1)

where, $\epsilon_i$ is the on-site potential at the $i$-th atomic site and $t_{ij}$ is the nearest neighbor hopping integral. $\theta_{ij} = 2\pi \Phi / \Phi_0$ is the Peierl’s phase which is included in the hopping along each arm of a hexagon. $\Phi_0 = hc/e$ is the fundamental flux quantum. With the selective inclusion of the
magnetic flux, the graphene-fractal now describes a system where the time reversal symmetry
is broken only on a subset of the bonds. Consequent changes in the energy spectrum and
transport characteristics thus need to be examined in details. It may be mentioned that, the
triangular symmetry underlying a graphene topology has been exploited previously by Vargas
and Naumis [24] to explain an increase in localization in a doped graphene. The present system
is thus worth examining.

Figure 1: Schematic diagram of a portion of the graphene-fractal scooped out of an infinite
graphene sheet. Each of the surviving hexagonal plaquettes is threaded by a uniform
magnetic flux $\Phi$. The underlying dotted line shows the Seirpinski gasket fractal geometry
in which the basic graphene-fractal geometry can be mapped onto by decimating the ‘B’
type (red) atomic sites.

For our purpose we shall consider constant values of $\epsilon_i = \epsilon_0$ and $t_{ij} = t_0$ throughout the
calculation. That is, the A- and the B-sites are not distinguished energetically. In the context
of the graphene sheet they are all carbon atoms.

The Schrödinger equation for the original graphene network is equivalently cast into a set of
difference equations, viz,

$$(E - \epsilon_i) \psi_i = \sum_j t_{ij} e^{i\theta_{ij}} \psi_j$$

which is utilized in decimating out a suitable subset of atoms to reduce the infinite graphene-
fractal to a standard triangular SPG. In this triangular SPG, there is a uniform value of the
effective on-site potential $\epsilon$, which, of course, is a function of energy now. The nearest neighbor
hopping integrals assume two different values depending on the phase associated with them.
The distribution is illustrated in Fig. 1(a). The bonds of the inner triangles are associated with
the hopping integrals $\tau_f$ (forward) and $\tau_b$ (backward), while those along the outer triangle are designated by $t_f$ and $t_b$ respectively. The values of these parameters are given by:

$$
\epsilon = \epsilon_0 + \frac{2t_0^2}{E - \epsilon_0}, \\
\tau_f = \frac{t_0^2e^{2i\theta}}{E - \epsilon_0}, \quad \tau_b = \frac{t_0^2e^{-2i\theta}}{E - \epsilon_0}, \\
t_f = \frac{t_0^2e^{-i\theta}}{E - \epsilon_0}, \quad t_b = \frac{t_0^2e^{i\theta}}{E - \epsilon_0}
$$

\[3\]

Figure 2: (a) Schematic diagram of the effective Seirpinski gasket fractal which is obtained by decimating the the ‘B’ type (red) atomic sites from the original graphene-fractal network. The arrows show the direction for forward hopping from one atomic site to another atomic site – for the inner triangles it is $\tau_f$ and for outer triangles it is $t_f$. (b) The renormalized version of (a).

The effective SPG network (Fig. 2a)) is easily renormalized (Fig. 2b)) and the renormalized values of the parameters are:

$$
\epsilon' = \epsilon + 2(ut_f + u^*t_b), \\
\tau'_f = vt_f + w^*t_b, \quad \tau'_b = wt_f + v^*t_b, \\
t'_f = vt_f + w^*t_b, \quad t'_b = wt_f + v^*t_b
$$

\[4\]
where, \( u = \frac{(p + rp^*)}{D}, \quad v = \frac{(q + rs^*)}{D}, \quad w = \frac{(s + rq^*)}{D} \)

\( u^* = \frac{(p^* + r^*p)}{D}, \quad v^* = \frac{(q^* + r^*s)}{D}, \quad w^* = \frac{(s^* + r^*q)}{D} \)

\( D = 1 - rr^* \)

Here, \( p = \frac{(E - \epsilon)t_b}{\delta_0}, \quad q = \frac{(E - \epsilon)t_f + \tau_b t_b}{\delta_0} \)

\( p^* = \frac{(E - \epsilon)t_f}{\delta_0}, \quad q^* = \frac{(E - \epsilon)t_b + \tau_f t_f}{\delta_0} \)

\( r = \frac{(E - \epsilon)\tau_f + (\tau_b)^2}{\delta_0}, \quad s = \frac{\tau_b t_f}{\delta_0} \)

\( r^* = \frac{(E - \epsilon)\tau_b + (\tau_f)^2}{\delta_0}, \quad s^* = \frac{\tau_f t_b}{\delta_0} \)

\( \delta_0 = (E - \epsilon)^2 - \tau_f \tau_b \)

The above set of recursion relations will now be analyzed to see the effects of a fractal distribution of holes in a graphene sheet with magnetic flux trapped in a selected set of the hexagons.

### 3. Results and discussion

#### 3.1 Local Density of States (LDOS) at the bulk atomic sites

We have calculated the LDOS at the ‘A’ type (black) bulk atomic sites for an infinite graphene-fractal using the Green’s function and a standard real space decimation technique [25]. The LDOS is given by,

\[
\rho_{00}(E) = \lim_{\eta \to 0} \left[ -\frac{1}{\pi} \text{Im} G_{00}(E + i\eta) \right] \tag{5}
\]

where, \( G_{00}(E) \) is the local Green’s function at the ‘A’ type (black) bulk atomic sites. To obtain \( G_{00} \), the recursion relations Eq. (4) are iterated with a small imaginary part added to the energy \( E \) until the magnitude of the nearest neighbor hopping goes to zero (or, equivalently, becomes less than a small pre-assigned quantity). The on-site potential flows to a fixed point value \( \epsilon^* \), and in this limit \( G_{00} = (E + i\eta - \epsilon^*)^{-1} \).
In the absence of any magnetic flux $\Phi$, the LDOS shows a fragmented structure (Fig. 3, top panel). Most of these fragmented states are localized states, which can be verified by studying the flow the hopping integral under successive iterations, keeping the energy at a particular value. With any arbitrarily chosen energy $E$ at which the LDOS is non-zero, the hopping integral flows to zero under RSRG steps.

Interestingly, such a graphene-fractal is found to sustain an infinite number of extended eigenstates. These eigenstates coexist with the localized states. This turns out to be a generic feature of the underlying triangular Sierpinski geometry [17, 18]. To extract such extended states we need to set the energy of the electron $E = \epsilon(\ell)$, where, $\epsilon(\ell)$ represents the effective on-site potential at a bulk atomic site after the $\ell$-th stage of renormalization. A look at the recursion relations given in Eq. (4) with $\Phi = 0$ will reveal that, setting $E = \epsilon(\ell)$ immediately leads to a ‘two-cycle’ fixed point, viz, $\epsilon(\ell+2) = \epsilon(\ell+1) = \epsilon(\ell)$ and $t(\ell+2) = -t(\ell+1) = t(\ell)$ beginning at a certain stage $\ell$ of renormalization. $E - \epsilon = 0$ gives a polynomial equation of $E$, the real solutions of which will yield the values of energies at which the states are extended. Of course, the solutions will have to lie within the spectrum of the graphene-fractal.

For example, if we set $E = \epsilon$ at the basic stage $\ell = 0$, with $\epsilon_0 = 0$, and $t_0 = 1$, then $E = \pm \sqrt{2}$ will be energies for two extended states sustained by the fractal lattice in the absence of any magnetic flux. If we set $E = \epsilon^{(1)}$ on a one step renormalized lattice and with zero flux, it leads to an equation,

$$E^6 - 8E^4 + 17E^2 - 10 = 0$$

The roots are, $E = \pm 1$, $\pm \sqrt{2}$, $\pm \sqrt{5}$. Out of these $E = \pm 1$ are ‘spurious’ roots, not included in the spectrum of the graphene-fractal, while the others are there, and correspond to two-cycle fixed points of the RSRG recursion relations beginning at the stage $\ell = 1$. These are extended eigenstates. It is to be noted that the roots evolving from the solution of the equation $E = \epsilon(\ell)$ are also included in the spectrum of $E = \epsilon(\ell+1)$. This is again a generic feature of the SPG [18].
Figure 3: Plots for Local Density of states (LDOS) with the energy of the electron \( (E) \) at the bulk atomic sites (‘A’ type) of an infinite graphene-fractal network for different values of magnetic flux \( \Phi \). (a) represents the case for \( \Phi = 0 \), (b) represents the case for \( \Phi = \Phi_0/4 \) and (c) represents the case for \( \Phi = \Phi_0/2 \). We have set \( \epsilon_0 = 0 \) and \( t_0 = 1 \).

3.1.2 The non-zero flux cases

(a) The general character of the spectrum:

As we set the magnetic flux \( \Phi \) in each hexagon to a non-zero value, continuous bands are seen to be created in the LDOS profile (Fig. 3 middle panel). In this we have shown the LDOS for \( \Phi = \Phi_0/4 \) and it clearly shows the continua in the range \( 1 < |E| < 2 \). In such continua the states are ‘extended’, as has been examined by picking up any energy in this domain arbitrarily, and studying the flow of the hopping integral. The hopping integral in general, oscillates chaotically

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and remain non-zero for an indefinite number of iterations. The LDOS profile shows a continuum zone for all non-zero values of $0 < \Phi < \Phi_0/2$. Energy eigenvalues, picked up arbitrarily from any such continuous zone, corresponds to an extended eigenstate of the system. The localized eigenstates are also there. The spectrum is a mixture of the bands of extended states and clusters of localized states. However, it is not apparent whether there is any possibility of a metal-insulator transition driven by the magnetic flux. At $\Phi = \Phi_0/2$ the fragmented character in the LDOS profile is restored again (Fig. 3 bottom panel).

(b) Fixed points:

In the presence of a magnetic flux, the extraction of a fixed point of the transformations Eq. (4) is a non-trivial issue. Nevertheless, it is possible to work out the case for $\ell = 1$. Setting $E = \epsilon^{(1)}$ leads to the equation,

$$f(E) = \cos 6\theta$$

(7)

where, $f(E) = (E^6 - 8E^4 + 17E^2 - 8)/2$ and $\theta = 2\pi\Phi/6\Phi_0$. Clearly, for any energy $E$ lying within the spectrum, whenever the left hand side of Eq. (7) remains bounded by $\pm 1$, one can tune the magnetic flux appropriately to satisfy the equation $E = \epsilon^{(1)}$. For this special value of the magnetic flux, a two- cycle fixed point behavior is obtained. We depict the variation of the

![Figure 4: Plot of energy function $f(E)$ on the LHS of Eq. (7) with energy $E$. The shaded portions under the curve shows the values of energy for which the value of $f(E)$ lies within $\pm 1$.](image-url)
left hand side of Eq. (7) in Fig. 4. In principle, any energy within the shaded zone (provided it is included in the overall energy spectrum) can be made to correspond to an extended eigenfunction by a magnetic flux, whose value can be estimated from Eq. (7). For example, if we set the Fermi level at $E = 0.7$ (in unit of $t_0$), then it can be worked out to find that a value of the magnetic flux $\Phi = 0.38178\Phi_0$ throws the parameter space $(\epsilon(\ell), t(\ell))$ into a two-cycle fixed point beginning at the $\ell = 1$. As soon as one shifts away from this special value of the flux, the hopping integrals usually flow to zero as the renormalization progresses. This implies that, once we fix the Fermi level at a special value, the entire graphene-fractal can be made to conduct or act as an insulator by tuning the magnetic flux piercing the elementary hexagons.

**(c) Flux controlled behavior of the eigenstates:**

Certain points are of interest, and need to be appreciated in the context of flux controlled behavior of the eigenstates in a graphene-fractal. To appreciate this discussion we first illustrate in Fig. 5 the variation of the LDOS against the magnetic flux at special values of energy $E = \sqrt{2}$ (Fig. 5(a)), and for $E = \sqrt{5}$ (Fig. 5(b)). In each diagram it is clear that the selected energy can be brought inside or thrown out of the energy spectrum by tuning the magnetic flux. We specially focus in and around $\Phi = \Phi_0/2$.

Let us first consider the case when $E = \sqrt{2}$. There is clearly a continuous distribution of flux values in the neighborhood of $\Phi = \Phi_0/2$, viz, for $0.495\Phi_0 < \Phi < 0.505\Phi_0$, for which the LDOS is non-zero. For this range of magnetic flux, with the selected energy, the hopping integral does not flow to zero, but becomes small and keeps on oscillating around a value $\sim 10^{-2}$. This implies that the wavefunction really does not decay, but the overlap of amplitudes at distant lattice sites becomes very small. This tempts us to categorize such states as **critical** [15], or at least they have very large localization lengths.

Choosing $E = \sqrt{5}$ leads to a more interesting scenario. We now have a sharply localized eigenstate for $\Phi = \Phi_0/2$. The LDOS is isolated at $\Phi = \Phi_0/2$, and is highly degenerate. Setting $E = \sqrt{5}$, and $\Phi = \Phi_0/2$ makes the hopping matrix element flow to zero quickly. This observation speaks in favor of the localized character of the states. Interestingly, in the immediate neighborhood of the center of the spectrum ($\Phi = \Phi_0/2$), the hopping integral displays non-zero
Figure 5: Variation of Local Density of States (LDOS) with the magnetic flux $\Phi$ at the bulk atomic sites (‘A’ type) of an infinite graphene-fractal network. (a) for energy $E = \sqrt{2}$ and (b) for energy $E = \sqrt{5}$. We have set $\epsilon_0 = 0$ and $t_0 = 1$.

values under successive iterations, indicating either completely extended states, or critical ones (in the sense as discussed above). We thus encounter a possibility of a reentrant crossover in the nature of the spatial extension of the wavefunction at $E = \sqrt{5}$ by tuning the magnetic flux around the half flux quantum.

3.2 Transmission characteristics of the finite graphene-fractal network

To get the two terminal end-to-end transmission coefficient for a finite sized graphene-fractal, we clamp the system between two semi-infinite ordered leads. The leads, in the tight binding
model, are described by a constant on-site potential $\epsilon_L$ and a nearest neighbor hopping integral $t_L$. We then successively renormalize the system to reduce it into an effective dimer (Fig. 6) consisting of two ‘renormalized’ atoms, each having an effective on-site potential equal to $\tilde{\epsilon}$ and with an effective hopping integral $\tilde{t}$.

Figure 6: Schematic diagram of the effective dimer clamped between two semi-infinite ordered leads.

The transmission coefficient across the effective dimer is given by [26]

$$T = \frac{4 \sin^2 ka}{[(M_{12} - M_{21}) + (M_{11} - M_{22}) \cos ka]^2 + [(M_{11} + M_{22}) \sin ka]^2}$$ (8)

where,

$$M_{11} = \frac{(E - \tilde{\epsilon})^2}{t_f t_L} - \frac{\tilde{t}_b}{t_L}, \quad M_{12} = -\frac{(E - \tilde{\epsilon})}{t_f}, \quad M_{21} = -M_{12}, \quad M_{22} = -\frac{t_L}{t_f}$$

and ‘a’ is the lattice constant and is taken to be equal to unity throughout the calculation.

In Fig. 7 (a), (b), and (c) we plot the two terminal transmission coefficient of a 4-th generation graphene-fractal for $\Phi = 0$, for $\Phi = \Phi_0/4$ and $\Phi = \Phi_0/2$ respectively. The figures bring out the typical fragmented spectrum for zero magnetic field, which then gets converted into patches of continua at $\Phi = \Phi_0/4$. Finally, at $\Phi = \Phi_0/2$, the fragmented character is restored, reflecting a poorly conducting system. These results are at par with our discussion about the general band structure of the graphene-fractal system.

We have also examined the AB oscillations in the transmission spectrum at particular values of the electron energy $E$. The oscillations have the typical $\Phi_0$ periodicity observed in systems even with a single loop. However, we do not show this result to save space.
Figure 7: Transmission coefficient across a 4-th generation graphene-fractal network for different values of magnetic flux $\Phi$. (a) represents the case for $\Phi = 0$, (b) represents the case for $\Phi = \Phi_0/4$ and (c) represents the case for $\Phi = \Phi_0/2$. We have set $\epsilon_0 = \epsilon_L = 0$ and $t_0 = t_L = 1$.

4. Concluding remarks

In conclusion, we have considered an infinite graphene sheet in which holes have been created following a Sierpinski fractal distribution. The electronic spectrum of the system, investigated within a tight binding Hamiltonian for spinless, non-interacting electrons reveal a wide variety in the nature of single particle states. The magnetic field piercing each basic hexagonal plaquette is shown to lead to absolutely continuous parts in the spectrum. The results are reflected in the flow of the hopping integrals, as observed within a real space renormalization group formalism. A crossover in the behavior of the wavefunction at particular values of the energy can be made.
to happen by tuning the magnetic flux. The graphene-fractal system is thus a candidate to be inspected more carefully as a potential electronic device.

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