On the extendedness of eigenstates in a hierarchical lattice: a critical view

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Abstract

We take a critical view at the basic definition of extended single particle states in a non-translationally invariant system. For this, we present the case of a hierarchical lattice and incorporate long range interactions that are also distributed in a hierarchical fashion. We show that it is possible to explicitly construct eigenstates with constant amplitudes (normalized to unity) at every lattice point for special values of the electron-energy. However, the end-to-end transmission, corresponding to the above energy of the electron in such a hierarchical system depends strongly on a special correlation between the numerical values of the parameters of the Hamiltonian. Keeping the energy and the distribution of the amplitudes invariant, one can transform the lattice from conducting to insulating simply by tuning the numerical values of the long range interaction. The values of these interactions themselves display a fractal character.

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1 Introduction

The problem of localization of single particle states that was initially raised and solved by Anderson and others [1] still remains very much alive [2, 3] and have given birth to an enormous and highly rich literature [4]-[13]. The fundamental result is that, in one and two dimensions all the single particle eigenstates are exponentially localized in presence of uncorrelated disorder [1], while in three dimensions one witnesses the possibility of a metal-insulator transition.

Interesting twist in the concept of electron localization in low dimensional systems came up with the work of Dunlap et al [6, 8] who discussed that a short range positional correlation between the constituents of a one dimensional disordered chain could lead to resonant (extended) eigenstates with high transmittivity. The basic cause was traced back to a local resonance in a cluster of impurities, and the case was referred to as the random dimer model (RDM). The idea was tested in low dimensions with various form of disorder by many others [9]-[11]. Later, it was argued, based on numerical diagonalization of the Hamiltonian that, suitable long range positional correlations between the potentials assigned to the atomic sites in a linear chain of atoms one could initiate a metal-insulator transition even in one dimension [12, 13].

The idea of generating extended eigenstates in low dimensional systems without any translational order (disordered systems provide one such class) was further extended to the infinite quasi-periodic chains, where one could unravel an infinite variety of these unscattered states owing to the self similarity of the lattices [14, 15]. Similar studies were carried out on fractal networks [16]-[20] where, even in the absence of any local resonating clusters such as in the case of the RDM [6] or in the case of a quasi-periodic chain [14] one finds an infinite number of extended single particle states. In fact, Schwalm and Moritz [20] have argued, based on an extensive numerical support that, even a continuum of extended eigenstates might exist in a class of fractal lattices, a possibility that was also pointed out earlier somewhere else [19].

In all these exciting conceptual developments, a critical issue is practically overlooked. This is the question of categorizing an extended (resonant) state. More explicitly, let us raise the question, “when do we call an eigenstate extended?” An obvious answer is obtained by looking at the amplitude of the wave function at a given energy. A non trivial distribution of the amplitude throughout an infinite lattice very legitimately points to an extendedness of the
eigenfunction. A second way to characterize an extended wave function is through a calculation of the electronic transmission across the lattice at the concerned energy. Usually, an extended state should give rise to a ballistic transmission. This second criterion is compatible to the first one in all systems where translational symmetry prevails. However, its not apparent whether these two demands always go hand in hand in systems where extended states exist even in the absence of any translational order (such as the fractals for example), and a serious introspection of the issue is in order.

In the present communication, we specifically address this problem. We provide explicit example of a hierarchical lattice with long range interactions where, eigenstates with identical (and non-zero) amplitudes can be constructed at all the lattice points for a special energy of the electron. This construction demands a well defined correlation between the numerical values of a subset of the Hamiltonian parameters. The energy of the electron can be chosen independent of all or, a sub-set of the hierarchical long range interactions. It is then shown that the corner-to-corner propagation of an electron depends crucially on the strengths of the long range interactions rendering, in some cases, the lattice completely transparent to an incoming electron. In other situations, with a different choice of the hierarchical parameter, a topologically identical lattice with the same constant distribution of amplitudes of the eigenfunction, becomes completely opaque to an electron with the same energy as in the first case. This observation, to our mind, introduces in a possible conceptual conflict between the extendedness of an eigenstate and a ballistic transmission, particularly in such hierarchical systems.

We discuss two kinds of hierarchical interaction in a fractal network designed in the line of the well known Berker lattice [21]. Hierarchical structures using superconducting wire networks have already been fabricated and studied experimentally [22]. With the present day nano-technology, tailor-made geometries with quantum dots are also possible to fabricate using scanning tunnel microscope(STM) as tweezers. Our proposed structures are therefore not far from reality. Also, by controlling the proximity of the dots one can induce tunnel hopping almost at will.

We work within a tight binding approach. A real space renormalization group (RSRG) decimation scheme [23] is employed to calculate the corner-to-corner electronic transmission in finite but arbitrarily large lattices, and to analyze the character of the electron states. Incidentally,
a similar analysis has been made recently [24] on a Koch fractal with hierarchical interactions, and similar questions have been raised. The present lattice is a non-trivial generalization of the Koch fractal[25], and exhibits a richer spectrum of results, yet maintaining the basic issue, viz., the nature of extended eigenstates in such fractal lattices.

In what follows, we describe the results. In section 2, we describe the model and the essential method in resolving the problem. Numerical results and related discussion are presented in section 3, and we draw our conclusions in section 4.

2 The model and the method

2.1 The Hamiltonian and the decimation scheme

We begin by referring to Fig. 1 and Fig. 2. We have designed a hierarchical lattice with two different configurations, in one of which the long range interaction is along the axial direction (Fig. 1) and in the other one, it is along the transverse direction (Fig. 2). We adopt a tight binding formalism, and incorporate only the nearest neighbor hopping. The tight binding Hamiltonian for non-interacting electrons in the Wannier basis is given by,

$$H = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{\langle ij \rangle} [t_{ij} |i\rangle\langle j| + t_{ji} |j\rangle\langle i|]$$ (1)

where, $\epsilon_i$ is the on-site potential of an electron on the $i$-th atomic site and $t_{ij} = t_{ji}$ is the nearest neighbor hopping integral between the $i$-th and $j$-th sites. For the nearest neighboring sites of the lattice we assume $t_{ij} = t$, while the long range hopping integrals are $t_{ij} = \tau$, and are assumed to follow a particular rule: $\tau(n) = \lambda^n t$ where, $n$ represents the level of hierarchy, and $\lambda$ is the hierarchy parameter. For such a hierarchical lattice of finite but arbitrarily large size, the on-site potential $\epsilon_i$ will be assigned values $\epsilon_A$ for the two extreme sites and $\epsilon_{B(n)}$, $\epsilon_{C(n)}$ etc. for the bulk sites depending on their positions on the lattice as explained in Fig. 1 and Fig. 2.

Exploiting to the self similarity of the lattice, we can apply the real space renormalization group (RSRG) decimation scheme [23] to decimate an appropriate subset of sites. In decimating those subset of sites, we have used the standard difference equation, which is an equivalent
description of the Schrödinger equation, viz.,

\[
(E - \epsilon_i) \psi_i = \sum_j t_{ij} \psi_j
\]  

(2)

Here, \(\psi_i\) is the amplitude of the wave function at the \(i\)-th atomic site and the index \(j\) represents the nearest neighbors of \(i\). The recursion relations for the site energies and hopping integrals for the two cases are given by:

**I. The axial case**

\[
\begin{align*}
\epsilon'_A &= \epsilon_A + \frac{\alpha t^2}{\beta(1 - \gamma^2)} \\
\epsilon'_{B(n)} &= \epsilon_{B(n+1)} + \frac{3\alpha t^2}{\beta(1 - \gamma^2)} \\
\epsilon'_{C(n)} &= \epsilon_{C(n+1)} + \frac{2\alpha t^2}{\beta(1 - \gamma^2)} \\
t' &= \frac{\alpha \gamma t^2}{\beta(1 - \gamma^2)} \\
\tau'(n) &= \tau(n+1) \quad \text{for all} \ n \geq 1
\end{align*}
\]  

(3)

where, \(\alpha = E - \epsilon_{C(1)}\), \(\beta = \alpha(E - \epsilon_{B(1)}) - 2t^2\) and \(\gamma = [2t^2 + \alpha \tau(1)] / \beta\)

(4)

**II. The transverse case**

\[
\begin{align*}
\epsilon'_A &= \epsilon_A + \frac{\delta \mu t^2}{(\mu^2 - 4t^4)} \\
\epsilon'_{B(n)} &= \epsilon_{B(n+1)} + \frac{3\delta \mu t^2}{(\mu^2 - 4t^4)} \\
\epsilon'_{C(n)} &= \epsilon_{C(n+1)} + \frac{2\delta \mu t^2}{(\mu^2 - 4t^4)} \\
t' &= \frac{2\delta t^4}{(\mu^2 - 4t^4)} \\
\tau'(n) &= \tau(n+1) \quad \text{for all} \ n \geq 1
\end{align*}
\]  

(5)
where, \( \delta = E - \epsilon_{C(1)} - \tau(1) \) and \( \mu = \delta[E - \epsilon_{B(1)}] - 2t^2 \)

We present our numerical results in the next section using the above set of recursion relations.

\[ 2.2 \text{ The transmission coefficient} \]

To get the end-to-end transmission coefficient of an \( \ell \)-th generation 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 \( \epsilon_0 \) and a nearest neighbor hopping integral \( t_0 \). We then renormalize the lattice \( \ell \) times to reduce it into an effective dimer consisting of the ‘renormalized’ \( A \)-atoms, each having an on-site potential equal to \( \epsilon_{A}^{(\ell)} \) and the effective \( A-A \) hopping integral \( t_{(\ell)}^{(\ell)} \). The transmission coefficient is then obtained by the well known formula \[26\],

\[ T = \frac{4 \sin^2 ka}{[(P_{12} - P_{21}) + (P_{11} - P_{22}) \cos ka]^2 + [(P_{11} + P_{22}) \sin ka]^2} \]  \hspace{1cm} (7)

where,

\[ P_{11} = \frac{[E - \epsilon_{A}^{(\ell)}] t_{(\ell)}}{t_0 t_{(\ell)}} - \frac{t_{(\ell)}}{t_0} \]
\[ P_{12} = -\frac{[E - \epsilon_{A}^{(\ell)}]}{t_{(\ell)}} \]
\[ P_{21} = -P_{12} \]
\[ P_{22} = -\frac{t_0}{t_{(\ell)}} \]  \hspace{1cm} (8)

Here, \( \cos ka = (E - \epsilon_0)/2t_0 \)

\( a \) is the lattice spacing in the leads, and throughout the calculation we shall set \( \epsilon_0 = 0 \), and \( t_0 = 1 \).
3 Numerical results and discussion

3.1 The eigenvalue spectrum

Before discussing the precise point of interest, we prefer to have a look at the eigenvalue spectra of the proposed hierarchical structures. In particular, we examine the formation of the bands and the gaps as a function of the hierarchy parameter $\lambda$ both for the axial and the transverse cases. To this end, we use a well known trick used frequently in the case of a quasi-periodic lattice [27], and later used for hierarchical structures as well [24, 28]. We sequentially generate periodic approximants of the original hierarchical structure, calculate the trace of the transfer matrix corresponding to a ‘unit cell’ and extract those values of energy for which the magnitude of the trace of the transfer matrix remains bounded by 2 [27]. The results are shown for the axial and the transverse cases in Figs. 3(a) and (b) respectively. The common feature in both the figures is the presence of multiple bands and gaps. A variation of the hierarchy parameter $\lambda$ leads to band overlapping. Specifically speaking, in the axial case, the density of allowed energy values is larger in the range $-0.2t \leq \lambda \leq 0.2t$. Band crossings maximize in this area. An increase in the numerical value of $\lambda$ leads to a thinning of the spectrum. Influence of $\lambda$ on the spectrum of the transverse model is also similar.

3.2 The unusual states

We now examine some special situation which is the focus of this article.

(a) The axial model

Let us begin with the axial model. It is easy to verify that, if we choose the energy of the electron $E = \epsilon_A + t$, then one can construct, by hand, a wave function with amplitude equal to unity at every lattice point, provided one also fixes

$$
\epsilon_{B(n)} + \tau(n) = \epsilon_A - 2t \\
\epsilon_{C(n)} = \epsilon_A - t \quad \text{for all } n \geq 1
$$

(9)
Two points are worth noting. First, the distribution of amplitude thus constructed is independent of the individual values of $\epsilon_{B(n)}$ and $\tau(n)$, and only requires the special correlation in their numerical values as suggested in Eq. (9). Thus, in principle, $\epsilon_{B(n)}$ can be chosen out of any sequence of uncorrelated random numbers. The values of the hopping integrals $\tau(n)$ only then need to be selected accordingly. Thus the constructed amplitude distribution remains valid even for a random choice of a subset of the on-site potentials $\epsilon_{B(n)}$, and presents a new kind of extended wave function. However, this construction can not automatically be related to the good transmission property of any large but finite lattice. This is easily understood when one appreciates that the choice of the energy didn’t depend on the hierarchically distributed hoppings viz., $\tau(n)$, but the end-to-end transmission is bound to be sensitive to the individual values of $\tau(n)$.

This is illustrated in Fig. 4(a), where we have worked out the transmission coefficient across a 7th generation hierarchical network and for $\tau(n) = \lambda \tau(n - 1)$, with $\tau(1) = \lambda t$. Energy is set at $E = \epsilon_A + t$. The corresponding eigenstate has equal amplitude (normalized to unity) at all lattice points. The transmission spectrum shows that the 7th generation network is transparent to an incoming electron with the above energy only when $\lambda$ assumes a specific set of values. The transmission in this range of $\lambda$ is completely ballistic for certain values. We may assign the wave function in this case the status of an extended state. Interestingly, the same distribution of the amplitudes of the wave function, at the same energy $E = \epsilon_A + t$ makes the lattice completely opaque to the incoming electron for other ranges of $\lambda$. The energy definitely corresponds to an eigenstate of the system, as has been verified by calculating the local density of states at the sites of an infinite hierarchical lattice for the axial case. Also, the very fact that, one is able to construct such a state on a lattice, no matter how large it is, automatically confirms that it is an eigenstate. This observation leads to the question of a proper identification of an extended state in a non-translationally invariant system.

The procedure can be implemented on say, a one step renormalized lattice. That is, we can extract an energy eigenvalue by solving the equation $E = \epsilon_A' + t'$. The energy turns out to be a function of $\epsilon_A$, $t$, $\epsilon_{C(1)}$, $\epsilon_{B(1)}$ and $\tau(1)$, but remains independent of $\epsilon_{B(n)}$, $\epsilon_{C(n)}$ and $\tau(n)$ for
\( n \geq 2 \). Once again we are to choose,

\[
\begin{align*}
\epsilon_{B(n)} + \tau(n) &= \epsilon'_A - 2t' \\
\epsilon_{C(n)} &= \epsilon'_A - t' \quad \text{for all } n \geq 2
\end{align*}
\]  

The entire scheme works as before. In Fig. 5(a) we illustrate the transmission coefficient for \( E = 0 \). This energy is extracted by solving the equation \( E = \epsilon'_A + t' \), where we have chosen \( \epsilon_A = \epsilon_{B(1)} = \epsilon_{C(1)} = 0 \), and \( t = \tau(1) = 1 \). A fine scan of a selected portion of Fig. 5(a) is presented in Fig. 5(b) to show the self similar distribution of the values of \( \lambda \). The process can, in principle, be continued and one can extract energy eigenvalues for such unusual eigenstates by solving the equation \( E = \epsilon_A^{(\ell)} + t^{(\ell)} \) at any \( \ell \)-th stage of renormalization. Ideally, we thus have an infinite number of such eigenstates.

(b) The transverse model

For the transverse model, we can use an identical string of arguments to construct an eigenstate with an amplitude equal to unity at every lattice point. For this construction we fix the energy \( E = \epsilon_A + t \), and demand,

\[
\begin{align*}
\epsilon_{B(n)} &= \epsilon_A - 2t \\
\epsilon_{C(n)} + \tau(n) &= \epsilon_A - t \quad \text{for all } n \geq 1
\end{align*}
\]  

This choice of parameters leads to a completely new scenario in comparison to the axial case. Here, for values of the hierarchy parameter \( \lambda > 1 \), it is found that at any \( \ell \)-th stage of renormalization the on-site potential at the \( C \)-sites grow following the rule:

\[
\epsilon^{(\ell)}_{C(n)} = \lambda \epsilon^{(\ell)}_{C(n-1)} - \xi^{(\ell)}(\lambda)
\]  

where, \( \xi^{(\ell)}(\lambda) \) is a constant, function of \( \lambda \), and the on-site potential at the \( B \)-sites at any \( \ell \)-th stage of renormalization \( \epsilon^{(\ell)}_{B(n)} \) remains constant. Thus an incoming electron with energy
$E = \epsilon_A + t$ will face effectively higher and higher potential barriers, offered by the ‘C’ sites while travelling through the lattice. This will lead to a gradual decay of the end-to-end transmission as the system grows in size. In the thermodynamic limit the hierarchical lattice will remain non-conducting. For $\lambda \leq 1$, no regular pattern in the on-site potentials is observed. However, the hopping integral $t$ always decays to zero for $E = \epsilon_A + t$.

We have also examined the case, where the energy is extracted from a one step renormalized lattice by solving the equation $E = \epsilon'_A + t'$. For this we are free to choose $\epsilon_A$, $\epsilon_{B(1)}$, $\epsilon_{C(1)}$, $t$ and $\tau(1)$ freely, that is, in an uncorrelated fashion. The correlation now sets in from the hierarchy level $n = 2$ onwards. For example, we have examined the special situation when $\epsilon_A = \epsilon_{B(1)} = \epsilon_{C(1)} = 0$, and $t = \tau(1) = 1$. The roots are, $E = -1.90321, 0.193937, \text{and } 2.70928$. The transmission in each case drops fast as the lattice grows in size. The amplitude-distribution on a one step renormalized lattice is such that $\psi_i = 1$ on every vertex of the renormalized lattice. Therefore, the states are still strictly localized. Thus we can say that, a hierarchically distributed long range hopping in the transverse direction does not allow the lattice to be conducting.

Thus, once we appreciate that a long range tunnel hopping can be associated with the proximity of the atoms in the structure, we see that a proximity along the principal axis of the fractal allows both for conduction and localization, whereas, a proximity in the transverse direction makes the lattice non-conducting in general.

Before we end, it should be emphasized that, all these discussions are made with reference to special values of the energy $E$ for which one can construct a unique spatially extended distribution of the eigenfunctions. However, hierarchical lattices, as already discussed in the introduction, may possess both localized and extended eigenstates coexisting in the spectrum. For example, we have worked out a special situation in the transverse case, where a different set of values for the Hamiltonian parameters and the electron-energy may lead to a one cycle fixed point of the parameter space. The eigenstate in this particular case is definitely extended and the transport is high. However, we refrain from entering into this aspect to save space.
4 Conclusions

In conclusion, we have undertaken a detailed study of the electronic states and transport across a hierarchical lattice corresponding to a special set of energy eigenvalues. The central issue has been to examine if an unambiguous definition of the extendedness of an eigenstate in a lattice that lacks translational symmetry is obtainable. We come to the conclusion that, a state that looks extended by construction is not necessarily conducting, and the mobility of the state is strongly sensitive to a correlated choice of a subset of the system parameters. Even within the same basic lattice topology, a long range correlated tunnel hopping along the principal axis is found to lead to both extended and localized states depending on the value of the hierarchy parameter. The hierarchically long range hopping in the transverse direction, on the other hand, makes the eigenfunction localized in the lattice.

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Figure Captions:

**Figure 1:** (Color online). (a) Schematic diagram of the 2nd generation of a hierarchical lattice with long range interaction along the ‘axial’ direction. ‘A’ denotes the extreme sites, while $B(n)$ and $C(n)$ represent the bulk sites depending on their positions in the lattice, $n$ being the hierarchy index. ‘$t$’ represents the nearest neighbor hopping integral and $\tau(n)$ represents the value of the long range hopping integral in the $n$-th level of hierarchy. (b) The renormalized version of (a).

**Figure 2:** (Color online). (a) Schematic diagram of the 2nd generation of a hierarchical lattice with long range interaction along the ‘transverse’ direction. ‘A’ denotes the extreme sites, while $B(n)$ and $C(n)$ represent the bulk sites depending on their positions in the lattice, $n$ being the hierarchy index. ‘$t$’ represents the nearest neighbor hopping integral and $\tau(n)$ represents the value of the long range hopping integral in the $n$-th level of hierarchy. (b) The renormalized version of (a).

**Figure 3:** (Color online). Energy eigenvalue spectrum of a hierarchical fractal lattice as a function of the hierarchy parameter $\lambda$, obtained from the trace of the transfer matrix for the 7th generation fractal, taken as the ‘unit cell’. We have set $\epsilon_A = \epsilon_B(n) = \epsilon_C(n) = 0$ with $n = 7$ and $t = 1$. (a) The axial case and (b) The transverse case.

**Figure 4:** (Color online). (a) Transmission coefficient across a 7th generation fractal network (the axial case) for $E = \epsilon_A + t$ with $\epsilon_B(n) + \tau(n) = \epsilon_A - 2t$, and $\epsilon_C(n) = \epsilon_A - t$. (b) Fine scan of a selected part of (a) to reveal the self-similar distribution of $\lambda$. We have set $\epsilon_A = 0$, and $t = 1$.

**Figure 5:** (Color online). (a) Transmission coefficient across a 7th generation fractal network (the axial case) for $E = \epsilon_A' + t'$ and (b) a fine scan of a selected part of (a) to reveal the self-similar distribution of $\lambda$. We have set $\epsilon_A = \epsilon_B(1) = \epsilon_C(1) = 0$, and $t = \tau(1) = 1$. 

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