A renormalization group analysis of extended electronic states in 1d quasiperiodic lattices

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ABSTRACT

We present a detailed analysis of the nature of electronic eigenfunctions in one-dimensional quasi-periodic chains based on a clustering idea recently introduced by us [Sil et al., Phys. Rev. B 48, 4192 (1993)], within the framework of the real-space renormalization group approach. It is shown that even in the absence of translational invariance, extended states arise in a class of such lattices if they possess a certain local correlation among the constituent atoms. We have applied these ideas to the quasi-periodic period-doubling chain, whose spectrum is found to exhibit a rich variety of behaviour, including a cross-over from critical to an extended regime, as a function of the hamiltonian parameters. Contrary to prevailing ideas, the period-doubling lattice is shown to support an infinity of extended states, even though the polynomial invariant associated with the trace map is non-vanishing. Results are presented for different parameter regimes, yielding both periodic as well as non-periodic eigenfunctions. We have also extended the present theory to a multi-band model arising from a quasi-periodically arranged array of $\delta$-function potentials on the atomic sites. Finally, we present a multifractal analysis of these wavefunctions following the method of Godreche and Luck [C. Godreche and J. M. Luck, J. Phys. A :Math. Gen. 23, 3769 (1990)] to confirm their extended character.

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I. Introduction

In the last decade there has been intense activity in theoretical studies of aperiodic lattices in one dimension. Apart from their intrinsic interest, these studies have been mainly motivated by the remarkable discovery of the so-called quasicrystalline ordering in solids, beginning with the work of Shechtman et al.\textsuperscript{1} in 1984. On the experimental side, one dimensional aperiodic lattices have also become interesting objects of study, following the successful fabrication of layered semiconducting superstructures grown epitaxially in accordance with the rules of the well-known Thue-Morse and Fibonacci sequences\textsuperscript{2}. Parallel with this development, theoretical studies have been made on a number of such one-dimensional systems for phonon, electron and magnon spectra\textsuperscript{3}. While most of these studies have been numerical, there have also been quite a few analytical attempts, starting with the pioneering work of Kohmoto et al.\textsuperscript{4} on the unusual electronic properties of the Fibonacci lattice.

The behaviour of the electronic eigenstates in one-dimensional lattices are well-known in the two extreme limits of random and perfect periodic ordering; in the former case all the eigenstates are localised, while in the latter they are extended. It is precisely because aperiodicity is a level of ordering intermediate between these two extreme limits that the electronic eigenstates in aperiodic linear systems often are found to be critical\textsuperscript{4}. Interestingly, there is also evidence for extended states in some of these systems\textsuperscript{5–9}. While the reason for the existence of critical states may be assigned to the lack of periodicity in these systems, extended states arise due to other reasons, as discussed below.

In a recent work\textsuperscript{5} we analysed this problem in one-dimensional systems and found that the basic reason may be traced to the existence of a particular type of correlation among the atoms in the lattice. For the sake of clarity we summarise here the main ideas developed in that work. In an elementary problem of Anderson localisation of the random distribution of $A$ atoms on a host lattice of $B$ atoms, it is well-known that there is an extended eigenstate at an energy $\epsilon_A$ in this system if the $A$ atoms always occur in pairs, that is as dimers. This is an instance of a definite kind of correlation leading to an extended state in a disordered system\textsuperscript{6}. In this case the correlation consists in the fact that an $A$ atom always appears as a member of a dimer. We may generalise this idea as follows. Consider the distribution of a certain well-defined cluster of atoms on a host lattice in one dimension. Suppose
that this cluster consists of a finite number of identical building blocks, each of which is a smaller unit consisting, in general, of several atoms. In the above example, for instance, a dimer may be regarded as a cluster of two consecutive $A$ atoms. If the building blocks are to be found only within the clusters and nowhere else on the lattice, then it can be shown that for certain energy values the contribution to the total transfer matrix for the chain from these clusters is unity. Therefore, at these special energies only the host lattice is effective in determining the electronic properties. If the host lattice is periodic, then there is a possibility of extended states at these energies for the whole system.

The special energies for which the states are extended are a property of the cluster only and do not depend on the lattice as a whole. Thus in our earlier example of random $AA$ dimers on a $B$ type host lattice, the special energy value $E = \epsilon_A$ is determined by considering the $AA$ cluster alone. Many other $1d$ lattices containing these $AA$ dimers may have an extended state at this same energy. To illustrate this let us consider a periodic lattice of $A$ atoms. Here the $AA$ correlation is trivially present, and therefore this system has an extended state at the same energy. However, while all eigenstates at energies other than $\epsilon_A$ are localised in the random dimer case, here we have a whole band of extended states, the existence of which cannot be inferred by considering the $AA$ dimers. Although Bloch’s theorem enables us to find this band directly, we may alternatively think of determining this band by considering higher order clusters consisting of triplets, quadruplets ... etc. of $A$ atoms, as has been discussed by us earlier. There is no advantage in adopting this point of view in this elementary example. However, in aperiodic chains Bloch’s theorem does not apply, and one has to use this idea in order to determine the bands or mini-bands of extended states.

The clusters contain only partial information about the entire lattice, and consequently, we have the same set of energy levels for systems all of which contain a particular cluster but which have different long-range compositions. The detailed differences in the electronic spectra in these systems are due to correlations at length scales beyond the cluster size. In order to bring out these differences we have to examine correlations among larger and larger blocks of atoms in the chain, by looking at the systems at increasing length scales. In this process the long range features of the lattice get gradually included and we end up by obtaining the entire spectrum of extended states. The real space renormalization group (RSRG) method is particularly suited
for studying this kind of problem.

In this paper we consider a period-doubling (PD) chain\textsuperscript{10,12} as a prototype example to illustrate the above clustering ideas. These ideas are quite general and are also applicable to other aperiodic systems. A PD chain, to our mind, is a very interesting candidate for investigation because the trace map associated with this chain leads to a polynomial invariant which is likely to ensure the critical nature of all the eigenstates as well as a Cantor set energy spectrum. As we will show in this paper, inspite of the existence of such an invariant, this lattice can sustain an infinity of extended eigenstates which coexist with the otherwise Cantor set nature of the energy spectrum.

The few analytical studies that are available on the PD lattice have all been made with a simple on-site tight-binding version of the lattice hamiltonian. Bellissard et al.\textsuperscript{11} have shown that the spectrum of a tight binding Schrodinger equation in which the potentials are distributed following a PD sequence is purely singular continuous and supported on a Cantor set of zero Lebesgue measure. In an earlier article Severin et al.\textsuperscript{12} analytically studied the case of a special class of quasiperiodic sequences generated by the substitution rule $S_{L+1} = S_{L-1}S_{L-1}S_L$ which yielded the standard copper mean lattice and variations of PD lattices on tuning the initial choice of the basic building blocks. They reported the existence of periodic eigenstates on such lattices at some special values of energy. From our point of view, the work of Severin et al. is particularly interesting, as they give an analytical method for locating the eigenvalues and the corresponding extended eigenstates for the PD sequence. The validity of their approach, however, is strictly limited to the use of the on-site model. Apart from this, their analysis crucially depends on a special choice of the value of the pseudo-invariant\textsuperscript{12} $\gamma$ for PD chain equal to 2, and it is not clear how this analysis can be extended to other values of $\gamma$.

Interestingly, in all the works on the PD chain reported so far, the clustering effect that we have discussed above, although present, has neither received adequate emphasis, nor has been made the focal point for analysing the nature of the eigenfunctions. As will be seen, the clustering idea enables us to reduce the problem of identification of the nature of eigenfunctions on any quasi-periodic lattice to its essential simplicity. Thus, for instance, by merely looking at the Fibonacci chain it is possible to infer that there are no extended states in general, without going into any further analytical consideration, since there is no clustering in this chain\textsuperscript{8}.
One of the aims of this paper is to investigate the nature and character of the electronic eigenfunctions with more general hamiltonians. Such an extension is necessary because any experimental realisation of a quasi-periodic chain will not be restricted to on-site variations of parameters only. As a first step we therefore look at a tight-binding model hamiltonian for the PD chain which includes simultaneous variations in both on-site and hopping matrix elements. This increase in the level of complexity is not readily amenable to analysis through the transfer matrix approach alone. For the PD case we find interesting cross-over behaviour in the nature of the eigenstates from an all states critical picture to a situation where we have an infinity of extended states, depending on the region of parameter space in which we work. We next consider the problem of the motion of an electron in an array of δ-function potentials whose strengths are distributed in accordance with the underlying quasi-periodicity of the lattice. This is a multi-band problem, and we find that the clustering idea still applies. We may regard this case as approximating the experimental situation more closely than the single band model based on the tight binding approach.

We organise this paper as follows. In the next section we give a somewhat detailed exposition of the clustering idea in the context of general single band tight binding models of a PD chain. We also present numerical results for the extended eigenfunctions obtained on the basis of the present theory. The extension to the multiband case is given in section III. Section IV deals with the multifractal analysis of the wave functions.

II. The Tight Binding Model

A portion of the period doubling chain is shown in Fig.1(a). The sequence in which the long (L) and short (S) bonds are arranged in this chain is obtained by successively using the substitution rule $L \rightarrow LS$ and $S \rightarrow LL$. For describing the electron states in this lattice we use the single band tight binding hamiltonian

$$H = \sum_i \epsilon_i |i><i| + \sum_{<ij>} t_{ij}|i><j|.$$  \hspace{1cm} (1)

Since we are interested in locating clustering effects at different length scales, it is essential to label the sites and the hopping matrix elements appropriately. This is necessary, because in order to implement the RSRG decimation scheme, the self-similarity inherent in the lattice has to be pre-
served at every stage of renormalization. Such labelling was discussed by us earlier for the Fibonacci lattice and the copper mean lattice\textsuperscript{5,8}. There is a basic difference in the renormalization procedure followed in the transfer matrix method and that in the present approach. Our approach is based on the global decimation procedure discussed by Southern et al.\textsuperscript{14}, in which we consider an infinitely long chain, and decimate a subset of sites so as to produce a self-similar chain on an inflated length scale. We find that we have to assign at least three different labels to the site energies and two to the hopping matrix elements to make this decimation possible in the PD chain. Consequently we identify three types of sites, which we label by $\alpha$, $\beta$ and $\gamma$ corresponding respectively to sites between two consecutive long ($L$) bonds, a long ($L$) bond and a short ($S$) bond, and a short ($S$) bond and a long ($L$) bond. The site energies in Eq.(1) therefore assume the values $\epsilon_\alpha$, $\epsilon_\beta$ and $\epsilon_\gamma$ respectively. The hopping matrix elements across the long bond ($L$) is taken as $t_L$ and that across the short bond ($S$) as $t_S$. As we shall see, the site energies and the hopping matrix elements of the renormalized chain at any stage carry these very five labels and no more. Of course later we shall discuss the very interesting case of a still more general model which has four types of hopping matrix elements across the long ($L$) bond depending on the vertices connected, and whose behaviour is quite different requiring a separate treatment.

Let us begin with the case where we have three site energies $\epsilon_\alpha$, $\epsilon_\beta$ and $\epsilon_\gamma$ and two hopping matrix elements $t_L$ and $t_S$. The eigenfunctions for such a lattice may be calculated by the standard transfer-matrix method. The Schrödinger equation for the hamiltonian (1) can be cast in the form $\phi_{n+1} = M_n \phi_n$, where

$$\phi_n = \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} \quad \text{and} \quad M_n = \begin{pmatrix} E - \epsilon_n & t_{n,n+1} \\ t_{n,n-1} & E - \epsilon_n \end{pmatrix}.$$ 

Here $\psi_n$ denotes the amplitude of the wave function at the $n$-th site and $M_n$ is a $2 \times 2$ transfer matrix. In the PD chain we have three different kinds of transfer matrices $M_\alpha$, $M_\beta$ and $M_\gamma$, and $\phi_n$ is related to $\phi_0$ by a product of these three matrices following the PD sequence.

By inspecting the PD chain (Fig.1(a)) we see that the $\alpha$-sites always occur in pairs whereas, the $\beta$ and $\gamma$ sites always occur as a doublet $\beta\gamma$. Thus for this lattice the pair of sites $\alpha - \alpha$ constitutes a cluster in the sense discussed in
the Introduction. For this chain the string of transfer matrices typically looks like \( \ldots M_{\beta\gamma} M_{\alpha} M_{\beta\gamma} M_{\beta\gamma} M_{\alpha} \ldots \), where \( M_{\beta\gamma} = M_{\gamma} M_{\beta} \). We notice that the matrix \( M_{\alpha} \) is unimodular. The pure on-site model results as a special case by taking \( \epsilon_\alpha = \epsilon_\gamma = \epsilon_A, \epsilon_\beta = \epsilon_B \) and \( t_L = t_S \) while the transfer model is obtained by taking \( \epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = \epsilon \) and \( t_L \neq t_S \).

Let us first discuss the general case of a one dimensional chain which contains \( m \)-component clusters, that is clusters each containing \( m \) identical building blocks. Let the transfer matrix for every building block be a \( 2 \times 2 \) unimodular matrix denoted by \( M \). The composite transfer matrix for the cluster is then \( M^m \). By a straightforward application of the Cayley-Hamilton theorem for the \( m \)-th power of a \( 2 \times 2 \) unimodular matrix \( M \) it can be shown that

\[
M^m = U_{m-1}(x)M - U_{m-2}(x)I \tag{2}
\]

where, \( x = (1/2)\text{Tr}M \). \( U_m(x) = \sin(m+1)\theta/\sin\theta \), with \( \theta = \cos^{-1} x \) is the \( m \)-th Chebyshev polynomial of the second kind\(^5\). For a value of the energy \( E \) for which \( U_{m-1}(x) \) becomes zero, \( M^m \) reduces to \( -U_{m-2}(x)I \), that is to say, the transfer matrix for this cluster behaves essentially as the identity matrix at this energy. Thus at this energy the entire lattice does not feel the presence of the cluster defined by the transfer matrix \( M^m \). If the remainder of the lattice forms a periodic chain, there will be extended states at this energy provided, this energy is an allowed one. For allowed states wave functions do not diverge at infinity.

For the PD chain \( M = M_\alpha \) and \( m = 2 \) and therefore setting \( U_1(x) = 0 \) we obtain \( E = \epsilon_\alpha \). For this energy the whole lattice effectively behaves as a periodic diatomic linear chain with each unit cell containing a \( \beta \) and a \( \gamma \) atom. If the energy \( E = \epsilon_\alpha \) happens to be within the allowed band of this diatomic lattice, then this energy is an allowed one. The condition for this is \((1/2)|\text{Tr}M_{\beta\gamma}| \leq 1\).

We now proceed to determine other energy eigenvalues which may give rise to extended eigenfunctions for the entire chain. From the Schrodinger equation for the PD chain (see Fig.1(a)) we obtain the following hierarchy of equations for the amplitudes of the wavefunction

\[
\begin{align*}
(E - \epsilon_\alpha)\psi_{-1} &= t_L\psi_0 + t_S\psi_{-2} \\
(E - \epsilon_\alpha)\psi_0 &= t_L\psi_1 + t_L\psi_{-1}
\end{align*}
\]
\begin{align*}
 (E - \epsilon_\alpha)\psi_1 &= t_L\psi_2 + t_L\psi_0 \\
 (E - \epsilon_\beta)\psi_2 &= t_S\psi_3 + t_L\psi_1 \\
 (E - \epsilon_\gamma)\psi_3 &= t_L\psi_4 + t_S\psi_2 \\
 &\vdots
\end{align*}

If we generate a renormalized PD chain by decimating an appropriate set of sites (see Fig.1(a)), then we obtain a self-similar hierarchy of equations, but with renormalized parameters corresponding to the inflated chain shown in Fig.1(a). The topology of the chain is preserved as a result of this transformation and the corresponding scale factor is two. The renormalized site energies and the hopping integrals are found to be

\begin{align*}
 \epsilon'_\alpha &= \epsilon_\gamma + \omega_\beta(t_L^2 + t_S^2) \\
 \epsilon'_\beta &= \epsilon_\gamma + \omega_\alpha t_L^2 + \omega_\beta t_S^2 \\
 \epsilon'_\gamma &= \epsilon_\alpha + (\omega_\alpha + \omega_\beta)t_L^2 \\
 t'_L &= \omega_\beta t_L t_S \\
 t'_S &= \omega_\alpha t_L^2
\end{align*}

where \(\omega_i = 1/(E - \epsilon_i), i = \alpha, \beta, \gamma\). Corresponding to this transformation it can be shown that there exists the following polynomial invariant

\[ I = \frac{(\epsilon_\alpha - \epsilon_\beta)(\epsilon_\alpha - \epsilon_\gamma) - t_L^2 - t_S^2}{2t_Lt_S} + 1, \]

whose value remains unchanged under the transformation Eq.(4), as can be easily verified. Since the renormalized chain is still a PD sequence, we again find \(\alpha\)-sites occurring as \(\alpha - \alpha\) pairs and \(\beta - \gamma\) sites forming \(\beta - \gamma\) doublets. This means that the \(\alpha - \alpha\) clustering effects are also present on this inflated length scale. With respect to this renormalized lattice there are extended eigenstates at \(E = \epsilon'_\alpha\) (when \(M^2_\alpha = -I\)), provided for this energy \(\kappa' = (1/2)|\text{Tr}M_{\beta\gamma}| \leq 1\), \(\alpha, \beta\) and \(\gamma\) now referring to the renormalized chain. Since the \(\alpha - \alpha\) clustering is present at every length scale, one will find, upon repeated renormalization, a number of extended state-energy eigenvalues by solving the equation \(E = \epsilon^{(n)}_\alpha\), and by checking that the roots of the equation satisfy the condition \(\kappa^{(n)} \leq 1\), where the trace \(\kappa^{(n)}\) is evaluated with the renormalized parameters at the \(n\)-th stage. Interestingly, for the PD chain...
we find that the value of $\kappa(n)$ becomes equal to $I - 1$ for energies which are the roots of the equation $E - \epsilon^{(n)}_\alpha = 0$, where, $I$ is the invariant defined in Eq.(5). This implies that $\kappa(n)$ is also independent of the generation index $n$ for these special energy values. Therefore, if the initial parameters are such that $\kappa(0)$ is greater than one, then there will be no extended states at any level of renormalization, and the roots of the equation $E - \epsilon^{(n)}_\alpha = 0$ will always be in the gaps of the entire band. On the other hand, if for the initial choice of parameters, $\kappa(0)$ is less than or equal to unity, then all the subsequent $\kappa(n)$’s will also be $\leq 1$, and thus all the solutions of the equation $E - \epsilon^{(n)}_\alpha(E) = 0$ will be allowed ones.

It is to be appreciated that the $\alpha - \alpha$ clustering at larger length scales amounts to including, so to say, the effects of larger and larger segments of the original chain into the $\alpha$-subclusters. The $\alpha - \alpha$ correlation at all length scales can only be revealed by renormalization group methods. While in the original lattice this correlation is directly visible (Fig.1(a)), higher order correlations due to $\alpha - \alpha$ pairing imply underlying complex correlations between atoms, which is not apparent from mere inspection of the original lattice.

With this background we are now in a position to discuss several models of the PD chain which are obtained by assigning different values to the hamiltonian parameters. Specifically, we shall discuss the following models:

(i) The on-site model

In this model the hopping matrix elements are all taken to be equal and the site energies are of two types, $\epsilon_A$ and $\epsilon_B$, arranged on a lattice following the PD sequence. Severin et al.12 in their analysis showed that this chain supports extended states which display periodicity of periods 4, 8 . . . etc. in units of lattice spacing. They made use of the fact that a pseudo-invariant associated with this model has a value equal to 2, which is then used to establish the periodic nature of the solutions. From our point of view, we recover the on-site model by putting $\epsilon_\alpha = \epsilon_\gamma = \epsilon_A$, $\epsilon_\beta = \epsilon_B$ and $t_L = t_S = t$. For numerical calculations we choose $\epsilon_A = 1$, $\epsilon_B = -1$, $t = 1$ in suitable units, which are the same as those used by Severin et al., in order to afford a comparison with their calculation. At the basic level the extended state occurs at $E = \epsilon_A = 1$, and the wavefunction for this energy is found by the transfer matrix procedure beginning with the value $\psi_1 = 1$ and $\psi_0 = 0$ for a 7th generation PD chain with 128 atoms. The wavefunction is shown in Fig.2(a) and is identical with that of Severin et al.12 having a periodicity of
4 units of lattice spacing. This energy value yields for the quantity $\kappa^{(0)}$ the value -1, corresponding to the edge of the unperturbed $\beta\gamma$ band of energies. Since this quantity equals $I - 1$, the trace values $\kappa^{(1)}, \kappa^{(2)}, \ldots$, are all equal to -1. If we now consider the renormalized chain, then the extended states occur at energies obtained from the equation $E - \epsilon'_\alpha(E) = 0$, the roots being $\pm \sqrt{3}$. The wavefunction for $E = \sqrt{3}$ is shown in Fig.2(b), with a period of 8 units, and is again identical with that of Severin et al.\cite{12} At the next level we have the energies by solving $E - \epsilon''_\alpha(E) = 0$, which yields the roots $E = -1.82595501$, -0.15244466, 1.38553731 and 2.59286237. In Fig.2(c) we give the wavefunction for $E = 2.59286237$. This function is seen to have a period of 16 units. Finally, in Fig.2(d) we plot the wavefunction for the energy $E = 2.60380559$, obtained from the next level of renormalization.

As was pointed out by Severin et al., the underlying reason for the observed periodicity of say, the eigenfunction corresponding to $E = 1$ having a period of four lattice spacings, is related to the vanishing of the amplitude at every fourth site on the chain. Alternatively, we note that at this energy, the hierarchy of Eqs.(3) are indistinguishable from that of an infinite periodic lattice of alternate $A$ and $B$ atoms. Similarly, the equations determining the eigenfunctions of period 8 are identical with that of an ordered lattice with unit cell consisting of $ABAA$ atoms. In the same manner it is found that every periodic solution in the on-site model is identical with the solution of some periodic chain with a suitable unit cell. Thus it turns out that in this case we may associate a whole array of periodic lattices with different unit cells with the extended eigenfunctions, each periodic lattice being in one to one correspondence with one of the eigenvalues of the PD chain. A similar observation has been made recently by Oh and Lee\cite{16}.

(ii) The transfer model

As mentioned before, the transfer model is obtained by choosing the starting values $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma$, and $t_L \neq t_S$. For numerical work we choose the values $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = 0$, $t_L = 1$ and $t_S = 2$. For this case the energy for the extended state $E = 0$ lies in the central gap of the band, with a value of $\kappa^{(0)} = -1.25$. Again, from the invariance of the trace under the RSRG transformation, it follows that $\kappa^{(n)} = -1.25$ for all $n$, that is, all the energy values are disallowed and thus there are no extended states in this model. In fact, in this model the value of $\kappa^{(n)}$ for any choice of $t_L$ and $t_S$ is of the form $\kappa^{(n)} = (1/2)(x + 1/x)$, where, $x = t_L/t_S$, and thus $\kappa^{(n)}$ is always greater
than unity. Since the value of $\mathcal{I}$ in this case is non-zero, the eigenstates are all critical supported on a Cantor set of zero measure.

(iii) The mixed model

Let us begin with the case where all the site energies are unequal, and there are two different hopping matrix elements $t_L$ and $t_S$. The transfer matrix $M_\alpha$ for this case is unimodular, and hence the energies for the extended states are again obtained from the equation $E - \epsilon_\alpha^{(n)}(E) = 0$. The band of energies allowed by the periodic $\beta\gamma$ chain defined by the initial parameters lies in the range

$$\left(\frac{\epsilon_\beta + \epsilon_\gamma + \sqrt{(\epsilon_\beta - \epsilon_\gamma)^2 + 4(t_S + t_L)^2}}{2}, \frac{\epsilon_\beta + \epsilon_\gamma + \sqrt{(\epsilon_\beta - \epsilon_\gamma)^2 + 4(t_S - t_L)^2}}{2}\right)$$

and

$$\left(\frac{\epsilon_\beta + \epsilon_\gamma - \sqrt{(\epsilon_\beta - \epsilon_\gamma)^2 + 4(t_S - t_L)^2}}{2}, \frac{\epsilon_\beta + \epsilon_\gamma - \sqrt{(\epsilon_\beta - \epsilon_\gamma)^2 + 4(t_S + t_L)^2}}{2}\right)$$

If the value of $\epsilon_\alpha$ lies outside these energy intervals, then $\kappa^{(0)}$ becomes greater than unity at the energy $E = \epsilon_\alpha$ and there is no extended state at any level of renormalization. With the progress of renormalization the periodic $\beta\gamma$ chains with renormalized parameters will yield more and more fragmented bands, and the energy values obtained as solutions of $E - \epsilon_\alpha^{(n)}(E) = 0$ will always be in the gaps of these fragmented spectrum. Since the value of $\mathcal{I}$ is non-zero, all the states will be critical even in the presence of $\alpha - \alpha$ clustering. On the other hand, if the value of $\epsilon_\alpha$ lies inside one of the initial energy intervals defined above, we always have $\kappa^{(n)} \leq 1$, and the states will be extended. The extended character of each wavefunction has been checked by a multifractal analysis (see section IV). There is thus a cross-over in the behaviour of the eigenstates depending on the choice of the initial parameters. Confining our attention to the regime of extended behaviour, we find an interesting systematics in the nature of the eigenfunctions as we consider the roots of $E - \epsilon_\alpha^{(n)}(E) = 0$ for increasing values of $n$. Choosing $\epsilon_\alpha = 4$, $\epsilon_\beta = 0$ and $\epsilon_\gamma = 3$, $t_L = 1$ and $t_S = 2$, we find that all the wavefunctions are non-periodic, as can be seen from Fig.(3), where we have displayed the eigenfunctions at the energies $4, -1.19258240, 5.45570651$ and $3.56527726$ arising from the
first four levels of renormalization. In Fig.(4) eigenfunctions are shown for energies $-0.60581006$, $4.14562305$, $4.65276530$ and $5.45820519$, which arise from the solution of $E - \epsilon^{(4)}_\alpha(E) = 0$. As may be seen, the amplitudes of these non-periodic functions do not decay as we go from one end of the chain to the other. We have tested the non-decaying character of the wavefunctions for chain lengths up to $2^{18}$ atoms, although we have presented the amplitudes for much smaller chain lengths for convenience. A very interesting feature that may be noted is that eigenfunctions corresponding to neighbouring energies possess, in general, entirely different profiles. This feature is contrary to what one obtains in a periodic lattice, and one may regard this behaviour as a manifestation of the quasiperiodic character of the lattice.

We now go on to the discussion of a still more general model, namely one in which, in addition to having three different site-energies, we ascribe four different values to the hopping integral across the long bonds connecting $\alpha\alpha$, $\alpha\beta$, $\gamma\alpha$ and $\gamma\beta$ pairs of sites. While the primary reason for considering this model is that it represents the realistic situation most closely within the framework of the single band nearest neighbour tight-binding hamiltonian, an additional reason is that even though $\alpha - \alpha$ clusters are seen to be present, the matrix $M_\alpha$ will have two different values depending on the immediate neighbours of an $\alpha$ site. Neither of these two $M_\alpha$ matrices is unimodular, and therefore one cannot apply the result of Eq.(2) to this case. Inspite of this, the present model gives rise to an infinity of extended states. To see this, if we consider only the subset of $\alpha$ sites in this PD chain, then these sites are found to form a lattice in which two different bond lengths are arranged in the copper-mean sequence. In the same manner, each of the subset of $\beta$ and $\gamma$ sites forms a copper-mean sequence. If we now decimate the original PD chain so as to retain only the $\beta$ sites (the same could have been done for the $\alpha$ or $\gamma$ sites), then we may relabel the sites of the resulting lattice following the prescription of the copper-mean chain discussed by us earlier, so that the original PD chain transforms into a copper mean lattice (see Fig.1(b)) with four site-energies $\epsilon^{CM}_\alpha$, $\epsilon^{CM}_\beta$, $\epsilon^{CM}_\gamma$ and $\epsilon^{CM}_\delta$ and two different hopping integrals $t^{CM}_L$ and $t^{CM}_S$ defined as

\begin{align*}
\epsilon^{CM}_\alpha &= \epsilon_\beta + st^2_\alpha \omega_\gamma + qt^2_{\alpha\beta} \omega_\alpha \\
\epsilon^{CM}_\beta &= \epsilon_\beta + t^2_\beta \omega_\gamma + qt^2_{\alpha\beta} \omega_\alpha \\
\epsilon^{CM}_\gamma &= \epsilon_\beta + st^2_\gamma \omega_\gamma + t^2_{\gamma\alpha} \omega_\gamma
\end{align*}

(6)
\[ \epsilon_{CM}^\delta = \epsilon_\beta + t_2^2 \omega_\gamma + t_{\gamma \alpha}^2 \omega_\gamma \]
\[ t_L^{CM} = p \ q \ t_\alpha t_\gamma t_\alpha \omega_\gamma \omega_\alpha^2 \]
\[ t_S^{CM} = t_{\gamma \alpha} \ t_\gamma \omega_\gamma, \]

where \( \omega_i \)'s have been defined previously. \( p, q, r \) and \( s \) are given by
\[ p = \left( 1 - t_{\gamma \alpha}^2 \omega_\alpha \omega_\gamma \right)^{-1} \]
\[ q = \left( 1 - p t_{\alpha \alpha}^2 \omega_\alpha^2 \right)^{-1} \]
\[ r = \left( 1 - t_{\alpha \alpha}^2 \omega_\alpha^2 \right)^{-1} \]
\[ s = \left( 1 - r t_{\gamma \alpha}^2 \omega_\alpha \omega_\gamma \right)^{-1}. \]

Very interestingly we find that as a result of this transformation the hopping matrix elements for the effective copper-mean chain takes only two different values depending on the two distinct bonds in this renormalized lattice, even though we had started with the most general version of the PD chain. In this renormalized copper-mean lattice we have again the \( \alpha - \alpha \) clustering as discussed in Ref.5, and this leads to a whole hierarchy of extended states, provided \( (1/2)|\text{Tr}(M_\gamma M_\beta)| \leq 1. \)

Two comments are in order at this stage. Firstly, it is impossible to discern this clustering effect at the level of the original PD chain, and the full spectrum of extended states can be obtained only through this initial transformation to a copper-mean lattice. This means, that the original PD chain does implicitly contain a complex clustering involving all the \( \alpha, \beta \) and \( \gamma \) sites, but which does not show up at the initial stage. Secondly, it may seem that one could have straightaway applied this transformation to any of the models discussed earlier. However, it should be appreciated that there is a basic difference between the RSRG transformation for a PD lattice and that for a copper-mean chain. While there exists a polynomial invariant \( I \) associated with the PD chain, there is no such invariant for the copper-mean case. The value of \( I \) for the most general model is found to be
\[ I = \frac{(E(t_{aa}^2 - t_{\gamma \beta}^2) - t_{aa}^2 \epsilon_\gamma + \epsilon_\alpha t_{\gamma \beta}^2)(\epsilon_\alpha - \epsilon_\beta) - t_\gamma t_{aa} t_\gamma (t_\alpha - 2t_{\alpha \beta}) - t_{aa}^2 t_{\gamma \beta}^2}{2t_\gamma t_{\gamma \beta} t_{aa}^2}. \]

(7)

In determining \( I \) we have set the initial hopping integrals \( t_{aa} = t_{aa} \) and \( t_{\gamma \alpha} = t_{\gamma \beta} \). This is, of course, not a restrictive condition, since starting with the most general model with four different values for the hopping integral.
for the long bonds, we get, upon decimating alternate sites following the PD renormalization rule, only two different values for this hopping, which we may choose to be $t_{\alpha\alpha}$ and $t_{\gamma\beta}$. The quantity $\mathcal{I}$ is a linear function of energy, in contrast to any of the other models discussed earlier. By setting $\mathcal{I} = 0$ (see Ref.7 and 8), we immediately find that there is an additional extended state at an energy

$$E = \frac{(\epsilon_\alpha - \epsilon_\beta)(\epsilon_\gamma t^2_{\alpha\alpha} - \epsilon_\alpha t^2_{\gamma\beta}) + t^2_{\alpha\alpha}(t_S - t_{\gamma\beta})^2}{(\epsilon_\alpha - \epsilon_\beta)(t^2_{\alpha\alpha} - t^2_{\gamma\beta})}.$$  \hfill (8)

We have computed this wavefunction numerically with $\epsilon_\alpha = 1$, $\epsilon_\beta = 0$, $\epsilon_\gamma = 0.1$, $t_{\alpha\alpha} = 1$, $t_{\gamma\alpha} = 1.1$ and $t_S = 2$, for which $E$ is found to have a value 1.428571428. This extended state cannot be detected from a consideration of the effective copper mean lattice. The character of this extended state is entirely different from the other extended states in the PD lattice, if one looks at the pattern of flow of the Hamiltonian parameters in the copper-mean chain with renormalization. As has been pointed out by us earlier\(^5\), for an energy obtained from the equation $E - \epsilon_{\alpha}^{(n)}(E) = 0$ for the effective copper-mean lattice, the values of $\epsilon_\beta$ and $\epsilon_\gamma$ become equal after a certain number of iterations depending on the value of $n$, and remain so in subsequent iterations. Moreover, the hopping integrals do not flow to zero, which is an evidence of the extended nature of these eigenfunctions. On the other hand, for the special energy value defined in Eq.(8), $\epsilon_\beta$ is never found to become equal to $\epsilon_\gamma$ at any stage of iteration, although the hopping integrals do remain finite and non-zero, indicating that this state is also extended. The chaotic behaviour of the flow pattern may be said to characterise this eigenstate. The corresponding wavefunction is shown in Fig.(5), and its extended character is confirmed through the multifractal analysis given in section (IV).

### III. The Multi-Band Model

Let us now consider the continuum version of the Schrödinger equation in one dimension with a quasi-periodic potential $V(x)$. We may transform this equation with any arbitrary potential to a discrete set of difference equations using the standard Poincare map\(^{13}\). If we label the points on a 1$d$ lattice by the integers $x_i$, then we can find a recursion relation for the amplitudes of the wavefunction at three consecutive points of the above set. In the usual language of tight binding theory, the “hopping matrix element” connecting
amplitudes on neighbouring points \( x_i \) can be expressed in terms of the Wronskian matrix corresponding to the solutions of the Schrödinger equation in that interval. We omit the expressions here and refer to the literature for details\(^\text{13}\). For simplicity, let us apply this theory to the case of an array of \( \delta \)-function potentials sitting at the sites \( i \) with strengths \( \lambda_i \) distributed according to the PD sequence. The Poincare map leads us to a set of difference equations of the following form connecting the amplitudes at three successive points:

\[
\psi_{n+1} + \psi_{n-1} = [2 \cos q + (\lambda_n/q) \sin q] \psi_n \tag{9}
\]

where \( q = \sqrt{(E)} \). Here \( \lambda_n \) gives the strength of the potential at the \( n \)-th site. The energy eigenvalues forming bands of extended states correspond to the values of the wave vector \( q \) satisfying the inequality

\[
2 \cos q + (\lambda_n/q) \sin q \leq 2 \tag{10}
\]

In order to extract information about the spectral nature as well as the character of the eigenfunctions in this case we can recast Eq.(9) in the following form:

\[
(E' - \epsilon_n)\psi_n = \psi_{n-1} + \psi_{n+1} \tag{11}
\]

with \( E' = 2 \cos q \) and \( \epsilon_n = -(\lambda_n \sin q)/q \). This is now in the familiar form of the single band tight binding hamiltonian where \( E' \) now plays the role of the ‘energy’ and \( \epsilon_n \) can be interpreted as the ‘effective’ on site potential distributed according to the PD sequence. We may now assign three different labels \( \alpha, \beta \) and \( \gamma \) to the sites of the chain and adopt the same procedure as described earlier for finding the extended eigenstates. Setting \( E' = \epsilon^{(n)}_\alpha \), where, \( n \) implies the \( n \)-th stage of renormalization, we have been able to locate the eigenvalues corresponding to the extended eigenfunctions for the multiband PD chain. There is however, an important aspect to note, viz. setting \( E' = \epsilon_\alpha \) even at the initial stage we arrive at an equation of the form

\[
2/\lambda_\alpha = -(1/q) \tan q. \tag{12}
\]

Now \( \tan q \) is a \( \pi \) -periodic function and it takes all values in the interval \(-\infty \to \infty\) for any value of \( \lambda_\alpha \). Therefore, at each stage of renormalization the solution of the equation \( E' = \epsilon^{(n)}_\alpha \) will give rise to an infinite countable set of energy eigenvalues for which the PD chain will be totally transmitting. That
is to say, we have infinite number of extended eigenfunctions at all scales of length. This result is to be contrasted with the case of a tight binding random dimer model which exhibits a resonance state at a unique energy, or with the results for the copper-mean chain or the PD chains in the tight binding versions where, at each stage of renormalization one generally enumerates a finite number of extended eigenstates. For numerical calculation of the wavefunctions we have taken $\lambda_\alpha = \lambda_\gamma = 1$ and $\lambda_\beta = -1$. At the very initial stage, by setting $E' = \epsilon_\alpha$ we obtain an infinite number of allowed $q$ values. We have explicitly calculated the wavefunction for $q = 1.836597203$ and the result is shown in Fig.6(a). This wavefunction is real and periodic with a period four. The amplitudes follow the sequence $1, 0, -1, 0$ for the first four sites and this pattern is repeated for the rest of the lattice. The discontinuity of the derivative of the wavefunction at lattice points $x = 3na$, $n = 1, 2, 3...$ have been shown encircled in Fig.6(a). From the next level of renormalization, we have chosen $q = 2.37738316$ from the set of allowed $q$-values, and have plotted the wavefunction, which has a periodicity of eight, in Fig.6(b). The wavefunctions for other levels of renormalization may be obtained in the same manner.

**IV. Multifractal Analysis of the Wavefunctions**

All the wavefunctions given in this paper have been subjected to a multifractal analysis to verify their extended nature. Following the standard procedure, a “partition function” is defined as

$$Z(Q) = \sum_{i=1}^{N} |\psi_i|^Q$$

where $N$ is the number of sample points. For sufficiently large $N$, $Z(Q)$ may be expressed as

$$Z(Q) = \epsilon^{\tau(Q)}$$

where $\epsilon$ is the interval $1/N$, and $\tau(Q)$ is an index from which the multifractal index $\alpha$ and the corresponding fractal dimension $f(\alpha)$ are obtained as

$$\alpha = \frac{d\tau(Q)}{dQ} \quad \text{and} \quad f(\alpha) = Q\alpha - \tau(Q).$$

As is known\textsuperscript{15}, the standard algorithm is however not of much practical utility unless the sample size is inordinately large. With all finite, reasonably
large, sample sizes one always obtains a distribution in the values of $\alpha$ and $f(\alpha)$. This is a finite-size effect and the convergence to the true behaviour occurs only logarithmically slowly with increase in the sample size\textsuperscript{15}. Thus the standard procedure cannot be regarded as a reliable method to analyse finite size samples. As has been explicitly shown by Godreche and Luck\textsuperscript{15}, a much better method to test the extended character is to look at the behaviour of the curvature of $\alpha - f(\alpha)$ curve at $Q = 0$. As has been shown by them, the quantity $|1/f''(\alpha)|_{Q=0}$, which is a measure of the curvature at the maximum of the $\alpha - f(\alpha)$ graph, should diverge linearly with log($N$) for extended states, $N$ being the sample size. On the contrary, if the given set is a true multifractal, the curvature should gradually saturate to single value with log($N$). In our case we have used this prescription to test our wavefunctions, with a maximum sample size of $2^{17}$ values of the amplitudes. In every case, we observe the predicted linearity in the dependence of $|1/f''(\alpha)|_{Q=0}$ with log($N$). In Fig.7 we give the results for three of the wavefunctions, including the ‘chaotic’ wavefunction shown in Fig.5, the graphs for all the other wavefunctions being entirely similar. Our analysis, therefore provides confirmatory evidence that the states obtained on the basis of the present work are true extended states.
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FIGURE CAPTION

Fig.1 (a) A section of the period-doubling chain. The $\alpha$, $\beta$ and $\gamma$ sites are indicated respectively by a full circle, a square and an open circle. $\alpha - \alpha$ clusters are shown encircled by dotted lines. The renormalized chain under a period-doubling decimation is also shown. (b) Effective copper-mean chain obtained by eliminating the $\alpha$ and $\gamma$ sites in the period-doubling chain. The $\alpha$, $\beta$, $\gamma$ and $\delta$ sites are marked by a full circle, square, open circle and a triangle in the copper-mean chain. $\alpha - \alpha$ clusters in the copper-mean chain are also indicated.

Fig.2 Wavefunctions for the period-doubling chain in the on-site model for $\epsilon_\alpha = \epsilon_\gamma = 1$, $\epsilon_\beta = -1$, $t_L = 1$ and $t_S = 2$. For (a) $E = 1$, (b) $E = \sqrt{3}$, (c) $E = 2.59286237$ and (d) $E = 2.60380559$. All energies are in units of $t_L$.

Fig.3 Wavefunctions for the period-doubling chain in the mixed model for $\epsilon_\alpha = 4$, $\epsilon_\beta = 0$, $\epsilon_\gamma = 3$, $t_L = 1$ and $t_S = 2$. For (a) $E = 4$, (b) $E = -1.19258240$, (c) $E = 5.45570651$ and (d) $E = 3.56527726$. All energies are in units of $t_L$.

Fig.4 Wavefunctions for the period-doubling chain in the mixed model. Parameters are the same as for Fig.(3). The energies are for (a) $E = -0.60581006$, (b) $E = 4.14562305$, (c) $E = 4.65276530$ and (d) $E = 5.45820519$.

Fig.5 Wavefunction for the general model : $\epsilon_\alpha = 1$, $\epsilon_\beta = 0$, $\epsilon_\gamma = 0.1$, $t_{\alpha\alpha} = t_{\alpha\beta} = 1$ and $t_{\gamma\alpha} = t_{\gamma\beta} = 0.1$, and $t_S = 2$, for $E = 1.428571428$ obtained from Eq.(8). The energies are in units of $t_{\alpha\alpha}$.

Fig.6 Wavefunctions for the period-doubling chain in the multi-band case for $\lambda_\alpha = \lambda_\gamma = 1$, $\lambda_\beta = -1$ for (a) $q = 1.836597203$ corresponding to a period four and (b) $q = 2.377380316$ for a period eight. The energies are measured in units such that $\hbar^2/2m = 1$. The discontinuities in $\psi'(x)$ are shown encircled.

Fig.7 Plot of $|1/f''(\alpha)|_{Q=0}$ (curvature) against log($N$) corresponding to wavefunctions in Fig.2(d), Fig.3(d) and Fig.5 are shown in (a), (b) and (c) respectively. The maximum sample size has been taken as $2^{17}$. 

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