Extended states in 1D lattices : application to quasiperiodic copper-mean chain

S. Sil, S. N. Karmakar, R. K. Moitra
Saha Institute of Nuclear Physics
1/AF Bidhannagar, Calcutta 700 064, India
and
Arunava Chakrabarti
Theory Group, H. H. Wills Physics Laboratory
Tyndall Avenue, Bristol, BS8 1TL, U.K.

PACS Nos. : 61.44.+p, 64.60.Ak, 71.20.Ad, 71.25.-s
Abstract

The question of the conditions under which 1D systems support extended electronic eigenstates is addressed in a very general context. Using real space renormalisation group arguments we discuss the precise criteria for determining the entire spectrum of extended eigenstates and the corresponding eigenfunctions in disordered as well as quasiperiodic systems. For purposes of illustration we calculate a few selected eigenvalues and the corresponding extended eigenfunctions for the quasiperiodic copper-mean chain. So far, for the infinite copper-mean chain, only a single energy has been numerically shown to support an extended eigenstate [You et al. (1991)] : we show analytically that there is in fact an infinite number of extended eigenstates in this lattice which form fragmented minibands.
In recent years extended electron states have been found in a variety of diverse 1D systems [1-14] ranging from disordered systems on the one hand to various kinds of quasiperiodic systems on the other. In most cases, such states are identified through extensive numerical computations [1-8]. A general analytical understanding of this problem is still lacking [9-14]. In this paper we like to address this problem and we wish to see under what physical conditions extended states are expected to occur in disordered or quasiperiodic systems.

Consider an elementary example – an Anderson localisation problem involving the random distribution of A atoms on a host B-atom lattice. It is well-known [3, 10] that there is an extended eigenstate at a certain energy in this system if the A-atoms always occur in pairs, i.e., in the form of dimers. This is an instance of a definite kind of correlation between atoms leading to extended states in a disordered system. In this case, the correlation consists in the fact that an A atom always occurs as a member of a dimer. We may generalise this idea as follows. Suppose that there is a certain cluster of atoms which is distributed in some manner on a linear chain. Let this cluster consist of a finite repitition of a certain subcluster of atoms. Thus in the above example, a cluster (an AA pair) is made up by repeating a subcluster (an A atom) a finite number (two) of times. If this subcluster is to be found only within the clusters and nowhere else in the chain, then it can be shown [12] that for certain discrete energy values these clusters offer identity contributions to the total transfer matrix [15]. At these special energies we may disregard the presence of the clusters themselves, and if it happens that the remaining part of the lattice is a periodic one, then evidently this lattice will support extended states at these energies.

The special energies which support extended states are a property of the cluster only, and do not depend on the lattice as a whole. Thus, in our example of randomly distributed A-type dimers on a B-type host lattice (RDL), the special energy value $E = \varepsilon_A$ at which there is an extended state is determined from the consideration of the AA cluster alone [12]. At this energy value these AA dimers make identity contributions to the total transfer matrix and the chain effectively consists only of B atoms. We now wish to emphasize that many other 1D lattices containing these AA dimers may have extended states at this same energy. We may illustrate this by considering an ordered chain consisting only of A atoms and comparing its spectrum with that of the RDL. In the ordered chain the AA correlation is trivially
present, and therefore this system supports an extended state at the same energy. However, and this the crucial point we wish to make, while all eigenstates at other energies are localised ones in the RDL, in the ordered chain of A atoms we have a whole band of extended states, the existence of which cannot be inferred from a consideration of the AA dimer alone. Although this band can be found directly by using Bloch’s theorem, we do encounter many systems also possessing bands or minibands of extended states [5-14], where this theorem cannot be used as there is no periodicity. An example of this is the quasiperiodic copper-mean chain (CMC).

The clusters contain only part of the information about the entire lattice, and therefore, provide a common set of energy levels for a variety of systems which contain these clusters but which otherwise differ among themselves in their long range behaviour. In general, these systems possess correlations beyond the level of what is contained in the clusters themselves, which are responsible for the detailed differences in electron spectra among them. 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 system at larger and larger length scales. In this process the long range features of the lattice, which may include periodicity, or may be self-similarity, get gradually included in the determination of the electronic spectra, and we end up by obtaining the entire spectrum of extended states.

In this paper we present an approach which incorporates this point of view for finding the full spectrum of extended states in 1D lattices, periodic, quasiperiodic or disordered. The most natural method of including the effects of correlations at all length scales is the real space renormalisation group (RSRG) method, which is adopted here.

Although the discussion so far has been perfectly general, from now on we illustrate our ideas by focussing attention on the CMC. A portion of a CMC is shown in Fig. 1. The sequence in which long (L) and short (S) bonds are arranged in a CMC may be obtained from the substitution rule $L \rightarrow LSS$ and $S \rightarrow L$ starting with, say, $L$. For describing the electron states in this lattice we use the tight binding hamiltonian

$$H = \sum_i \varepsilon_i |i\rangle\langle i| + \sum_{<ij>} t_{ij} |i\rangle\langle j|$$

(1)

As shown in Ref. [7], for implementing the RSRG method in CMC we have to identify four types of sites, namely, $\alpha$, $\beta$, $\gamma$ and $\delta$ corresponding
respectively to the \(L-L, L-S, S-L\) and \(S-S\) vertices (Fig. 1). The site energies in Eqn.(1) assume the values \(\varepsilon_\alpha, \varepsilon_\beta, \varepsilon_\gamma\) and \(\varepsilon_\delta\), and there are two different values of the nearest neighbour hopping integrals, \(t_L\) and \(t_S\).

The eigenfunctions for such an 1D lattice may be calculated by the standard transfer-matrix method \[15\]. The discretized Schrödinger equation can be cast in the form \(\phi_{n+1} = M_n \phi_n\), where

\[
\phi_n = \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} \quad \text{and} \quad M_n = \begin{pmatrix} \frac{E-\varepsilon_n}{t_{n,n+1}} & -\frac{t_{n,n-1}}{t_{n,n+1}} \\ \frac{t_{n,n-1}}{t_{n,n+1}} & \frac{E-\varepsilon_{n-1}}{t_{n-1,n}} \end{pmatrix}.
\]

Here \(\psi_n\) denotes the amplitude of the wavefunction at the \(n\)-th site and \(M_n\) is a \(2 \times 2\) transfer matrix. In the CMC, \(\phi_n\) is related to \(\phi_0\) by a product of four types of transfer matrices \(M_\alpha, M_\beta, M_\gamma\) and \(M_\delta\) following the copper mean sequence.

By inspecting the CMC (Fig. 1) we see that the \(\alpha\)-sites always occur in pairs, whereas, \(\beta, \gamma\) and \(\delta\) always form a triplet \(\beta\delta\gamma\). Thus, for this lattice, the pair of sites \(\alpha\alpha\) constitutes a cluster. If we now renormalise the lattice by applying the deflation rule \[8\] \(LSS \rightarrow L\) and \(L \rightarrow S\), we get a scaled version of the original lattice with scale factor \(\sigma = 2\). In the renormalised chain we again find \(\alpha\) sites occurring as \(\alpha\alpha\) pairs, and \(\beta, \gamma\) and \(\delta\) sites forming \(\beta\delta\gamma\) triplets. This means that the \(\alpha\alpha\) clustering effects are also present on this inflated length scale, and therefore, by induction, present at all length scales. It is important to appreciate that the \(\alpha\alpha\) clustering at larger length scales amounts to subsuming, so to say, the effects of larger and larger segments of the original chain into the \(\alpha\) subclusters, thereby allowing larger and larger portions of the chain to contribute to the special energies for the extended states.

It is clear from the above discussion that the \(\alpha\alpha\) correlation at all length scales can only be revealed by renormalisation group methods. While in the original lattice, this correlation is directly visible (Fig. 1), higher order correlations due to renormalised \(\alpha\alpha\) pairs imply underlying complex correlation between atoms, which is not apparent from mere inspection of the original lattice.

In a copper-mean lattice the string of transfer matrices typically looks like,

\[
\cdots M_{\beta\delta\gamma}M_\alpha^2M_{\beta\delta\gamma}^3M_\alpha^2M_{\beta\delta\gamma} \cdots,
\]

where, \(M_{\beta\delta\gamma} = M_\gamma M_\delta M_\beta\).
We notice that the matrix $M_{\alpha}$ is unimodular, and so we can apply a well-known result, due originally to Cayley and Hamilton, for the $m$-th power of a $2 \times 2$ unimodular matrix $M$:

$$M^m = U_{m-1}(x)M - U_{m-2}(x)I$$

(3)

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. Let the matrix $M^m$ correspond to the transfer matrix of a cluster composed of $m$ identical subclusters, each described by a $2 \times 2$ unimodular transfer matrix $M$. For a value of the energy $E$ for which $U_{m-1}(x)$ becomes equal to zero, we have $M^m = -U_{m-2}(x)I$, that is to say, the transfer matrix for this cluster behaves essentially as the identity matrix at this energy. Thus at this energy, the lattice does not ‘feel’ the presence of the clusters defined by the transfer matrix $M^m$. If the remainder of the lattice forms a periodic chain, there will be an extended state at this energy provided this energy is an allowed one. For allowed states wavefunctions do not diverge at infinity [15].

For the CMC, therefore, we have to put $m = 2$ in Eqn.(3). We see that $U_1(x) = 0$ for $E = \varepsilon_{\alpha}$, and therefore, for this energy $M_{\alpha}^2 = -I$ as $U_0(x) = 1$. Thus, for this energy, the string of transfer matrices given by Eqn. (2) is composed only of matrices $M_{\beta \delta \gamma}$. This effectively describes an ‘ordered’ linear chain composed of unit cells each containing three types of atoms $\beta$, $\delta$ and $\gamma$. Now, if the condition $(1/2)|\text{Tr}M_{\beta \delta \gamma}| \leq 1$ is satisfied for $E = \varepsilon_{\alpha}$, then this energy is an allowed one (see Ref.[15]), and we shall have an extended eigenstate for the whole system.

To determine all the other extended states, let us now consider all the successive renormalised versions of the original chain. The self-similarity of the lattice implies that one can apply the considerations discussed so far in this paper to every such renormalised version. At any stage $\ell$ of renormalisation, extended states will be found at energies for which $E = \varepsilon_{\alpha}^{(\ell)}$, where $\varepsilon_{\alpha}^{(\ell)}(E)$ is the renormalised site-energy of $\alpha$ site at this stage. The expression for $\varepsilon_{\alpha}^{(\ell)}$ can be obtained by iterating the recursion relations [7]

$$\varepsilon'_{\alpha} = \varepsilon_\gamma + Q(t_L^2P_\beta + t_S^2P_\delta), \quad \varepsilon'_{\beta} = \varepsilon_\gamma + Qt_S^2P_\beta, \quad \varepsilon'_{\gamma} = \varepsilon_\alpha + Qt_L^2P_\beta, \quad \varepsilon'_{\delta} = \varepsilon_\alpha, \quad t'_L = Qt_S^2t_LP_\betaP_\delta, \quad t'_S = t_L,$$

(4)

where $Q = (1 - t_S^2P_\beta P_\delta)^{-1}$ and $P_i = (E - \varepsilon_i)^{-1}$, with $i = \alpha, \beta, \gamma, \delta$. For the CMC, therefore, we have to put $m = 2$ in Eqn.(3). We see that $U_1(x) = 0$ for $E = \varepsilon_{\alpha}$, and therefore, for this energy $M_{\alpha}^2 = -I$ as $U_0(x) = 1$. Thus, for this energy, the string of transfer matrices given by Eqn. (2) is composed only of matrices $M_{\beta \delta \gamma}$. This effectively describes an ‘ordered’ linear chain composed of unit cells each containing three types of atoms $\beta$, $\delta$ and $\gamma$. Now, if the condition $(1/2)|\text{Tr}M_{\beta \delta \gamma}| \leq 1$ is satisfied for $E = \varepsilon_{\alpha}$, then this energy is an allowed one (see Ref.[15]), and we shall have an extended eigenstate for the whole system.

To determine all the other extended states, let us now consider all the successive renormalised versions of the original chain. The self-similarity of the lattice implies that one can apply the considerations discussed so far in this paper to every such renormalised version. At any stage $\ell$ of renormalisation, extended states will be found at energies for which $E = \varepsilon_{\alpha}^{(\ell)}$, where $\varepsilon_{\alpha}^{(\ell)}(E)$ is the renormalised site-energy of $\alpha$ site at this stage. The expression for $\varepsilon_{\alpha}^{(\ell)}$ can be obtained by iterating the recursion relations [7]
The roots of the polynomial \( E - \varepsilon_\alpha^{(\ell)} \) for every \( \ell \) yield a new set of energy values for which eigenstates are extended. The number of allowed energy values increases with the progress of iteration. The totality of all these energies constitutes the entire spectrum of extended states for the CMC. These energies form minibands in energy space, the existence of which was only detected previously through numerical work [7].

The CMC may be divided into three sublattices \( \Omega_1, \Omega_2 \) and \( \Omega_3 \) (Fig. 1), each being a scaled version of the original lattice [7]. The recursion relations in Eqn.(4) actually represent renormalisation of the original chain to the \( \Omega_1 \) sublattice. We can define similar RSRG transformations for the \( \Omega_2 \) and \( \Omega_3 \) sublattices. Let us denote the transformations for these three sublattices by \( T_1, T_2 \) and \( T_3 \). Previously we have determined \( \varepsilon_\alpha^{(\ell)} \) by applying \( T_1 \) transformation \( \ell \) times successively. In general \( \varepsilon_\alpha^{(\ell)} \) is to be determined by applying a string of \( \ell \) operators consisting of \( T_1, T_2 \) and \( T_3 \) in any arbitrary sequence.

A string of \( T \)'s represents a genealogical path in the sense of Ref.[16], and all the extended eigenstates corresponding to a given string of \( T \)'s can therefore be considered as members of the same ‘family’. These states are characterised by the same length scale, and they belong to the same point on the genealogical tree. Now it may happen that the states belonging to the same family appear in different regions of the energy spectrum, that is, they may belong to different minibands. In other words, two neighbouring states belonging to a small energy interval \( \Delta E \) may belong to entirely different families. This indicates that the minibands are composed of extended states which are, in general, characteristically different from each other, forming dense sets of discrete energies.

We now present some results of our calculations for the CMC. Taking the hamiltonian parameters as \( \varepsilon_\alpha = \varepsilon_\beta = \varepsilon_\gamma = \varepsilon_\delta = 0 \), and \( t_S/t_L = 2 \), the first few stages of renormalisation yield the extended state energy eigenvalues \( E^{(0)} = 0 \), \( E^{(1)} = \pm 3 \), \( E^{(2)} = \pm 1.3637980258 \) and \( \pm 3.0232523786 \), and so on. Only the case \( E^{(0)} = 0 \) has been detected earlier [8] through numerical calculations. In Fig. 2 we have displayed wavefunctions for a 20th generation copper-mean lattice consisting of 699051 bonds. The first column of Fig. 2 shows the amplitudes on the first 450 sites of this chain, for three selected energy values belonging to three different genealogies. The next column in this figure shows the amplitudes on the last 450 sites on this chain, for the same three energy values. Examining across a row we notice that the ‘local pattern’ of the wavefunction is the same throughout the chain, with the am-
plitudes oscillating in an aperiodic manner within definite bounds without
decaying, unlike the behaviour displayed by a critical or localised eigenfunc-
tion. The pattern itself is different for the three different rows. Although
these states are extended, they are not Bloch-like. For $E = 0$ Gumbs and
Ali [17] found that the amplitudes decay with a power law. However our
analysis and explicit evaluation of the wavefunction clearly shows that their
conclusion is incorrect.

As has been shown in an earlier work [11], in a quasiperiodic lattice the
flow pattern for the hamiltonian parameters under renormalisation at energy
eigenvalues for extended states displays a regularity which is absent in the
non-extended case. In the CMC, this regularity associated with an extended
state shows up in the site energies for the $\beta$ and $\gamma$ sites becoming equal, after
a certain step of iteration, the equality being maintained in all subsequent
steps. The level at which the $\beta$ and $\gamma$ site energies become equal for the first
time depends on the energy value. Furthermore, this level is the same for all
energy eigenvalues belonging to the same family.

The ideas discussed in this paper are very general. Thus an ordered chain
of A atoms ($\varepsilon_i = \varepsilon$ and $t_{ij} = t$)

may be regarded as consisting entirely of AA dimers, which remains true
at all subsequent length scales upon renormalisation of the chain. At any
level, say $n$, of iteration the energy eigenvalues are given by the following
analytical expression

$$E^{(n)} = \varepsilon \pm t\sqrt{2 \pm \sqrt{2 \pm \sqrt{2 \pm \cdots}} \text{n times.}}$$  \hspace{1cm} (5)

The eigenvalues $E^{(0)}$, $E^{(1)}$, $E^{(2)}$, $\ldots$ $E^{(\infty)}$ taken together constitute the entire
band ranging from $\varepsilon - 2t$ to $\varepsilon + 2t$. The same approach applies to the
binary ordered chain of A and B atoms. Here again, the band edges and the
band gap extending from $\varepsilon_A$ to $\varepsilon_B$ due to the level repulsion are correctly
located. The problem of a random distribution of dimers on a lattice has
been already discussed, there being a single energy at which there is an
extended state. This is related to the fact that there is no deeper level of
correlation in this chain than what is contained through the existence of
dimers. If a disordered chain possess higher order correlations among the
sites in the sense discussed in this paper then there exist extended state at
several energies. This may explain the various observations reported in the
literature on disordered systems [1-4].
References

[1] J. B. Pendry, J. Phys. C 20, 733 (1987)

[2] M. Ya. Azbel, Phys. Rev. B 28, 4106 (1983); M. Ya. Azbel and P. Soven, Phys. Rev. B 27, 831 (1983); see also M. Ya. Azbel, Sol. St. Comm. 37, 789 (1981) and V. I. Mel’nikov, JETP Lett. 34, 450 (1981)

[3] D. H. Dunlap, H. L. Wu and P. Phillips, Phys. Rev. Lett. 65, 88 (1990); H. L. Wu, W. Goff and P. Phillips, Phys. Rev. B 45, 1623 (1992)

[4] T. J. Godin and R. Haydock, Phys. Rev. B 38, 5237 (1988)

[5] M. Kolar and M. K. Ali, Phys. Rev. B 39, 426 (1989)

[6] G. Y. Oh, C. S. Ryu and M. H. Lee, J. Phys.: Condens. Matter 4, 8187 (1992)

[7] Arunava Chakrabarti and S. N. Karmakar, Phys. Rev. B 44, 896 (1991)

[8] J. Q. You, J. R. Yan, T. Xie, X. Zeng and J. X. Zhong, J. Phys.: Condens. Matter 3, 7255 (1991)

[9] V. Kumar and G. Ananthakrishna, Phys. Rev. Lett. 59, 1476 (1987); V. Kumar, J. Phys.: Condens. Matter 2, 1349 (1990)

[10] X. C. Xie and S. Das Sarma, Phys. Rev. Lett. 60, 1585 (1988); S. Das Sarma, He Song and X. C. Xie, Phys. Rev. B 41, 5544 (1990)

[11] Arunava Chakrabarti, S. N. Karmakar and R. K. Moitra, Phys. Lett. A 168, 301 (1992)

[12] J. X. Zhong, T. Xie, J. Q. You and J. R. Yan, Z. Phys. B : Condensed Matter 87, 223 (1992)

[13] M. Severin and R. Riklund, Phys. Rev. B 39, 10362 (1989)

[14] M. Dulea, M. Severin and R. Riklund, Phys. Rev. B 42, 3680 (1990)

[15] M. Kohmoto, B. Sutherland and C. Tang, Phys. Rev. B 35, 1020 (1987)
[16] S. N. Karmakar, Arunava Chakrabarti and R. K. Moitra, Phys. Rev. B 46, 3660 (1992)

[17] G. Gumbs and M. K. Ali, J. Phys. A : Math. Gen. 22, 951 (1989)
Figure captions:

Fig.1 The $\alpha$ and $\beta\delta\gamma$ blocks in the copper-mean chain and also in its sublattices.

Fig.2 The amplitudes of the eigenfunction on the first 450 sites and the last 450 sites of a 20th generation CMC having 699051 bonds. Here $\varepsilon_\alpha = \varepsilon_\beta = \varepsilon_\gamma = \varepsilon_\delta = 0$ and $t_S/t_L = 2$. The 1st, 2nd and 3rd rows correspond to $E = 0$, $-1.3637980258$ and $-2.6255768195$ respectively. All energies are measured in units of $t_L$. We choose the boundary condition as $\psi_0 = 0$ and $\psi_1 = 1$. 