LETTER TO THE EDITOR

Extended electronic states in a Fibonacci chain

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Abstract. The electronic structure of a one-dimensional binary alloy $A_{1/\tau}B^2_{1/\tau}$ (with τ being the golden mean) with atoms A and B distributed in a Fibonacci sequence is studied using a tight-binding model, in which variation in both the diagonal and the off-diagonal terms is treated simultaneously. In contrast to the previous diagonal and off-diagonal models, for the 'mixed' model we find an extended state. Also in the limiting case of the 'off-diagonal' model the state corresponding to $E = 0$ is an extended state. These extended states are found to be independent of the arrangement of BA and BAA sequences in the Fibonacci chain.

The electronic structure of a Fibonacci chain ABAAB . . . has been widely studied in recent years [1, 2] using the tight-binding model

$$(E - \varepsilon_n)\Psi_n = t_{nn+1}\Psi_{n+1} + t_{nn-1}\Psi_{n-1}. \tag{1}$$

Almost all of these studies focus on two models: (i) the diagonal model where the site energy ε_n is assumed to take two values ε_A and ε_B according to whether the site is occupied by an A or a B atom in the Fibonacci chain with all the hopping integrals t_{nn+1} taken to be equal, and (ii) the off-diagonal model where $\varepsilon_n = 0$ for all n and t_{nn+1} takes two values t_A and t_B where A (B) now represents the long (short) bond in the Fibonacci sequence (FS). The energy spectrum in these models is a Cantor set and the wavefunctions are either self-similar or chaotic [3, 4]. In an actual alloy, however, both the terms will vary. In particular, in a simple model the hopping terms will take different values depending upon the chemical nature of the two species, so that in addition to the variation in ε_n, the hopping integral can take two values t_{AA} or t_{AB} ($=t_{BA}$) depending upon whether the nearest neighbour sites are occupied by identical or different atoms. Here we consider this 'mixed' model and show that an extended state can exist which depends upon the values of the parameters ε_N, t_{AA} and t_{AB}. Extended states in FS have been reported earlier [2] for the case where the cells contain more than one A or B atom. However, it was later pointed out [5] that extended states exist for such blocks of atoms irrespective of the sequence of the blocks. Therefore our result that extended state can exist without blocks of atoms is significant for a proper understanding of the properties of Fibonacci sequences of realistic systems.

1349

We first present the formalism and the results. We use the method of transfer matrices and introduce the transfer matrix

$$\mathbf{T}_n = \begin{pmatrix} (E - \varepsilon_n)/t_{nn+1} & -t_{nn-1}/t_{nn+1} \\ 1 & 0 \end{pmatrix} \tag{2}$$

so that equation (1) can be rewritten as

$$\begin{pmatrix} \Psi_{n+1} \\ \Psi_n \end{pmatrix} = \mathbf{T}_n \begin{pmatrix} \Psi_n \\ \Psi_{n-1} \end{pmatrix}. \tag{3}$$

Now consider the long-period structures corresponding to the Fibonacci sequences AB, ABA, ABAAB, ABAABABA, ... These can also be written in terms of the sequences BA, BAA, BAABA, BAABABAA, ... In the following the latter will be referred to as FS. Then the transfer matrices for the successive sequences can be obtained from the recursion relation

$$\mathbf{M}_j = \mathbf{M}_{j-2}\mathbf{M}_{j-1} \qquad j \geq 4 \tag{4}$$

where $\mathbf{M}_j$ represents the transfer matrix for the F_jth FS. Explicitly, $\mathbf{M}_2$ and $\mathbf{M}_3$ are given by

$$\mathbf{M}_2 = \begin{pmatrix} (E - \varepsilon_B)/t_{AB} & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} (E - \varepsilon_A)/t_{AB} & -1 \\ 1 & 0 \end{pmatrix} \tag{5}$$

and

$$\mathbf{M}_3 = \begin{pmatrix} (E - \varepsilon_B)/t_{AB} & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} (E - \varepsilon_A)/t_{AB} & -t_{AA}/t_{AB} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} (E - \varepsilon_A)/t_{AA} & -t_{AB}/t_{AA} \\ 1 & 0 \end{pmatrix}. \tag{6}$$

If $x_j = \frac{1}{2}\mathrm{Tr}(\mathbf{M}_j)$, then, as has been shown by Kohomoto and co-workers [1], the trace of the transfer matrix satisfies the recursion relation

$$x_{j+1} = 2x_{j-1}x_j - x_{j-2}. \tag{7}$$

This leads to the trace map for which

$$I = x_j^2 + x_{j+1}^2 + x_{j+2}^2 - 2x_j x_{j+1} x_{j+2} - 1 \tag{8}$$

is a constant. In our case this quantity is given by

$$I = [R(E - \varepsilon_A) - (E - \varepsilon_B)/R]^2/4t_{AB}^2 \tag{9}$$

where $R = t_{AB}/t_{AA}$. One can see that for the diagonal model this reduces to the result obtained earlier [2]. An interesting result is that in the present general case we can get an 'extended'-type state when I becomes zero. This happens for

$$E = \varepsilon_A(R^2 + 1)/(R^2 - 1) \tag{10}$$

where the origin of the energy is chosen such that $\varepsilon_B = -\varepsilon_A$. One limiting solution of equation (10) is $\varepsilon_A = E = 0$, which corresponds to the off-diagonal model in which $E = 0$ is an eigenvalue. Therefore in our off-diagonal model the centre of the band corresponds to an extended state. This is in striking contrast to the off-diagonal model studied by others, where the centre of the band has a self-similar wavefunction [1]. The
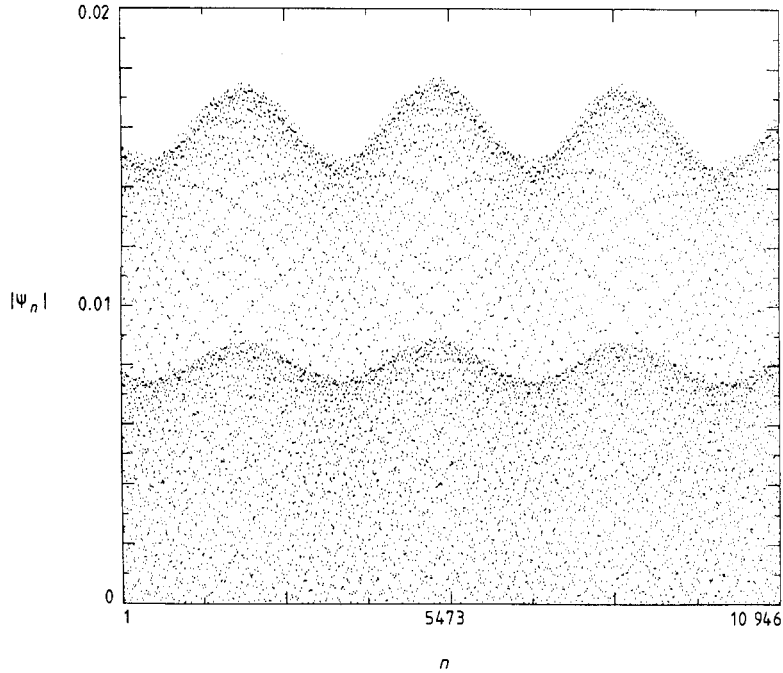
Figure 1. Normalised wavefunction for a Fibonacci chain of 10946 atoms for $E = -0.8$. $\varepsilon_B = -\varepsilon_A = 0.5|t_{AA}|$, $t_{AA} = -1.0$, $t_{AB} = -2.0$, $\Psi_0 = \Psi_{-1} = 1$.

extended state has very similar features to that studied by Kumar and Ananthakrishna [2]. The transfer matrices themselves have a six cycle and are given by

$$M_2 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \qquad M_3 = \begin{pmatrix} 0 & R \\ -1/R & 0 \end{pmatrix} \qquad M_4 = \begin{pmatrix} 0 & -R \\ 1/R & 0 \end{pmatrix}$$

$$M_5 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad M_6 = \begin{pmatrix} 0 & -R \\ 1/R & 0 \end{pmatrix} \qquad M_7 = \begin{pmatrix} 0 & -R \\ 1/R & 0 \end{pmatrix}. \tag{11}$$

It is clear that M_2 is a unit matrix and therefore for larger sequences the transfer matrix is a product of transfer matrices M_3. This is a situation analogous to the problem studied in [2]. Therefore the extended state remains even for arbitrary sequences of BA and BAA. Moreover $(M_3)^2$ is also -1. Therefore

$$\begin{pmatrix} \Psi_{n+1} \\ \Psi_n \end{pmatrix} = (-1)^p (-1)^{(q-r)/2} (M_3)^r \begin{pmatrix} \Psi_n \\ \Psi_{n-1} \end{pmatrix} \tag{12}$$

where p (q) is the number of M_2 (M_9) matrices in the product and r is 1 (0) if q is odd (even). Thus the wavefunction has a simple form and takes on values ± 1, $\pm R$ or $\pm 1/R$ if $\Psi_0 = \Psi_{-1} = 1$. It is easy to verify that even on the intermediate sites the wavefunction has one of these values. The A sites have $|\Psi_n|^2 = 1$ or R^2, whereas the B sites have $|\Psi_n|^2 = 1$ or $1/R^2$. The two values for A or B sites occur an equal number of times. By using multi-fractal analysis [6] it has recently been shown [3] that such extended type wavefunctions have $f(\alpha) = \alpha = 1$ as in the case of periodic systems. In the present case also it is very easy to show this.

We normalise the wavefunction for N sites and calculate the quantity

$$\sum_{i=1}^{N} |\Psi_i|^{2Q} = N^{(1-Q)} \frac{2^{Q-1}}{(1 + R^2/\tau + 1/R^2\tau^2)^Q} (1 + R^{2Q}/\tau + 1/\tau^2 R^{2Q}). \tag{13}$$

It is now easy to see that in the limit $N \to \infty$ the generalised dimension $D(Q)$ defined as

$$D(Q) = \ln \left(\sum_{i=1}^{N} |\Psi_i|^{2Q} \right) \Big/ (Q - 1) \ln(1/N) \tag{14}$$

becomes 1 for all Q. Therefore $\tau(Q) = \alpha Q - f = (Q - 1)$. $D(Q)$ gives $f(\alpha) = \alpha = 1$.

The general case given by equation (10) corresponds to the main point of this letter. Here the transfer matrices have no simple form such that a unit matrix could be found. The wavefunction has therefore been calculated numerically for a chain of 10 946 atoms with $\varepsilon_A = -0.5|t_{AA}|$ and $t_{AB} = 2t_{AA}$. Here t_{AA} has been taken to be -1. The normalised wavefunction is shown in figure 1 and is clearly of the extended type. We expect that in this case also $f(\alpha)$ and α should be equal to unity, but the analytical calculation will be difficult if not impossible. Also we expect certain bounds on the values of ε_A and R for this extended state to exist, such that the extended state falls within the allowed energy range. In the limiting case of $R \to 1$ there is no extended state, as is known. An interesting point to be noted here is that

$$[M_2, M_3] = [R(E - \varepsilon_A) - (E - \varepsilon_B)/R]/t_{AB} \begin{pmatrix} -1 & (E - \varepsilon_B)/t_{AB} \\ 0 & 1 \end{pmatrix}$$
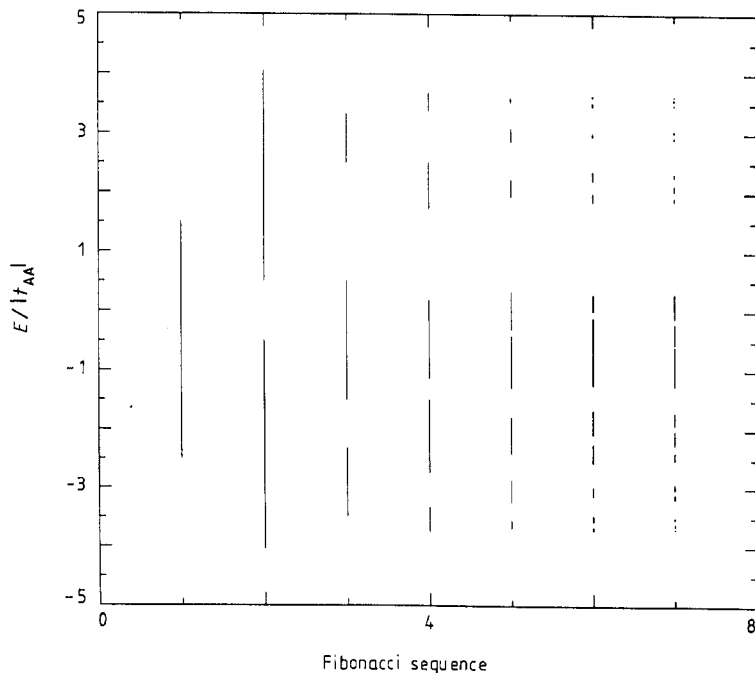
Figure 2. Energy spectrum for successive Fibonacci sequences for the same values of the parameters as in figure 1. 1, 2, . . . correspond to A, BA, . . . sequences. $t = t_{AA}$.

which vanishes for $I = 0$. Therefore the extended state in the mixed model still remains even if the BA and BAA sequences are interchanged.

The energy spectrum for successive Fibonacci sequences is shown in figure 2. As in the cases of the 'diagonal' and 'off-diagonal' models, it is a Cantor set. For the extended state at $E = -0.8|t_{AA}|$ the gap vanishes. Also, in the vicinity of the extended state other gaps are quite small. In the case of blocks of atoms the nature of states in the vicinity of the extended state has been studied in detail by Ananthakrishna and Kumar [3]. The crossover from extended to chaotic states is found to be gradual. In the present cases also we expect similar features.

In conclusion, we have shown that an extended state can exist for the 'mixed' model on the Fibonacci chain. This should be important for a proper understanding of the physical properties of Fibonacci superlattices. We also showed that the existence of the extended state is independent of the sequence of BA and BAA. It would be interesting to study the nature of other states in random sequences of BA and BAA. Also, in the case of more than one orbital per site a similar situation may arise and it can lead to the existence of other extended states. The vibrational spectrum of the Fibonacci chain where both the mass and the force constant variations are taken into account also has an extended mode and these results are presented elsewhere [7].

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