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ABSTRACT

The electronic structure of a one–dimensional binary alloy $A_{1/\tau}B_{1/\tau^2}$ (τ = golden mean) with A and B atoms distributed in a Fibonacci sequence is studied using a tight binding model in which the variation in both the diagonal and off–diagonal terms is treated simultaneously. In contrast to the previous 'diagonal' and the '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.

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

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

Almost all of these studies focus on two models. (1) 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} being taken equal and (2) the 'off-diagonal' model where $\varepsilon_n = 0$ for all n and t_{nn+1} takes on 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 on 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 occpied by identical or different atoms. Here we consider this 'mixed' model and show that there can exist an extended state depending 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 atoms. However, it was later pointed out [5] that for such blocks of atoms extended states exist 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.

We use the method of transfer matrices and introduce the transfer matrix

$$\underline{T}_n = \begin{pmatrix} \frac{E - \varepsilon_n}{t_{n,n+1}} & -\frac{t_{n,n-1}}{t_{n,n+1}} \\ 1 & 0 \end{pmatrix} \qquad (2)$$

so that Eq.(1) can be rewritten as

$$\begin{pmatrix} \Psi_{n+1} \\ \Psi_n \end{pmatrix} = \underline{T}_n \begin{pmatrix} \Psi_n \\ \Psi_{n-1} \end{pmatrix} \qquad (3)$$

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

$$\underline{M}_j = \underline{M}_{j-2}\, \underline{M}_{j-1} \qquad \text{for} \quad j \geq 4 \qquad (4)$$

where $\underline{M}_j$ represents the transfer matrix for the F_j^{th} FS. Explicitly $\underline{M}_2$ and $\underline{M}_3$ are given by

$$\underline{M}_2 = \begin{pmatrix} \frac{E - \varepsilon_B}{t_{AB}} & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{E - \varepsilon_A}{t_{AB}} & -1 \\ 1 & 0 \end{pmatrix} \qquad (5)$$

and

$$\underline{M}_3 = \begin{pmatrix} \frac{E - \varepsilon_B}{t_{AB}} & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{E - \varepsilon_A}{t_{AB}} & -\frac{t_{AA}}{t_{AB}} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{E - \varepsilon_A}{t_{AA}} & \frac{t_{AB}}{t_{AA}} \\ 1 & 0 \end{pmatrix} \qquad (6)$$

If $x_j = 1/2\ \mathrm{tr}(\underline{M}_j)$ then as shown by Kohomoto et al [1], the trace of the transfer matrix satisfies the recursion relation

$$x_{j+1} = 2\, x_{j-1}\, x_j - x_{j-2} \,. \qquad (7)$$

This leads to the trace map for which

$$I = x_j^2 + x_{j+1}^2 + x_{j+2}^2 - 2\, x_j\, x_{j+1}\, x_{j+2} - 1 \qquad (8)$$

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

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

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

$$E = \varepsilon_A\,(R^2 + 1)/(R^2 - 1) \qquad (10)$$

where the origin of the energy is chosen such that $\varepsilon_B = -\varepsilon_A$.

One limiting solution of Eq.(10) is $\varepsilon_A = E = 0$ which corresponds to the off-diagonal model for which $E = 0$ is an eigenvalue for all non-zero values of hopping integrals. Therefore in our off-diagonal model the center of the band corresponds to an extended state. This is in striking contrast to the off-diagonal model studied by others where the center of the band has a self-similar wavefunction [1]. The extended state

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

$$\underline{M}_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad \underline{M}_3 = \begin{pmatrix} 0 & R \\ 1/R & 0 \end{pmatrix} \quad , \quad \underline{M}_4 = \begin{pmatrix} 0 & -R \\ 1/R & 0 \end{pmatrix}$$

$$\underline{M}_5 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \quad \underline{M}_6 = \begin{pmatrix} 0 & -R \\ 1/R & 0 \end{pmatrix} \quad , \quad \underline{M}_7 = \begin{pmatrix} 0 & -R \\ 1/R & 0 \end{pmatrix} \qquad (11)$$

It is clear that $\underline{M}_2$ is a unit matrix and therefore for larger sequences the transfer matrix is a product of transfer matrices $\underline{M}_3$. This is a situation analogous to the problem studied in Ref.[2]. Moreover $\underline{M}_3^2$ is also -1. Therefore

$$\begin{pmatrix} \Psi_{n+1} \\ \Psi_n \end{pmatrix} = (-1)^p \, (-1)^{(q-r)/2} \, (\underline{M}_3)^r \begin{pmatrix} \Psi_n \\ \Psi_{n-1} \end{pmatrix} \qquad (12)$$

where p(q) is the number of $\underline{M}_2$ ($\underline{M}_3$) matrices in the product. r is 1(0) if q is odd(even). Thus the wavefunction has a simple form and takes on values ± 1, ± R or ± 1/R if $\Psi_0 = \Psi_{-1} = 1$. It 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 at equal number of times. Recently it has been shown [3] using the multifractal analysis [6] that such extended type wavefunctions have $f(\alpha) = \alpha = 1$ as in the case of periodic systems. In the present case it is also very easy to show this.

We normalize the wavefunction for N sites and calculate the quantity

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

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

$$D(Q) = \frac{\ln \left[\sum_{i=1}^{N} |\Psi_i|^{2Q} \right]}{(Q-1) \ln (1/N)} \qquad (14)$$

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 Eq.(10) corresponds to the main point of this article. 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 10946 atoms with $\varepsilon_A = -0.5\,|t_{AA}|$ and $t_{AB} = 2\,t_{AA}$. Here t_{AA} has been taken to be -1. The normalized wavefunction is shown in Fig.(1) and is clearly of 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 the existence of this extended state 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 it is known. The energy spectrum for successive Fibonacci sequences is shown in Fig.(2). As in the 'diagonal' and the '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 case 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. It would be interesting to study a model with more than one orbital per site where similar situation may arise and it can lead to the existence of other extended states. Also we expect the vibrational spectra of the Fibonacci chain where both the mass and the force constant variations are taken into account to show similar features.

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FIGURE CAPTIONS

Fig. 1. Normalized Wavefunction for a Fibonacci chain of 10946 atoms for E = -0.8. $\varepsilon_B = -\varepsilon_A = 0.5|t_{AA}|$, $t_{AA} = -1.0$, $t_{AB} = -2.0$, $\Psi_0 = \Psi_{-1} = 1$.

Fig. 2. Energy spectrum for successive Fibonacci sequences for the same values of the parameters as in Fig. 1. 1,2,... correspond to A, BA,... sequences. $t = t_{AA}$.

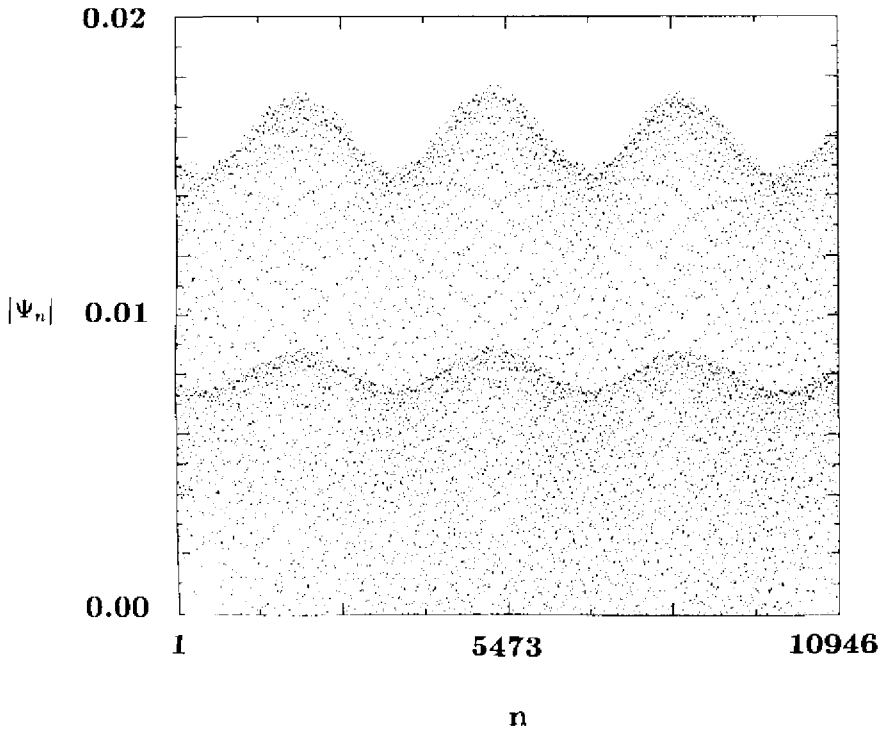

Fig.1

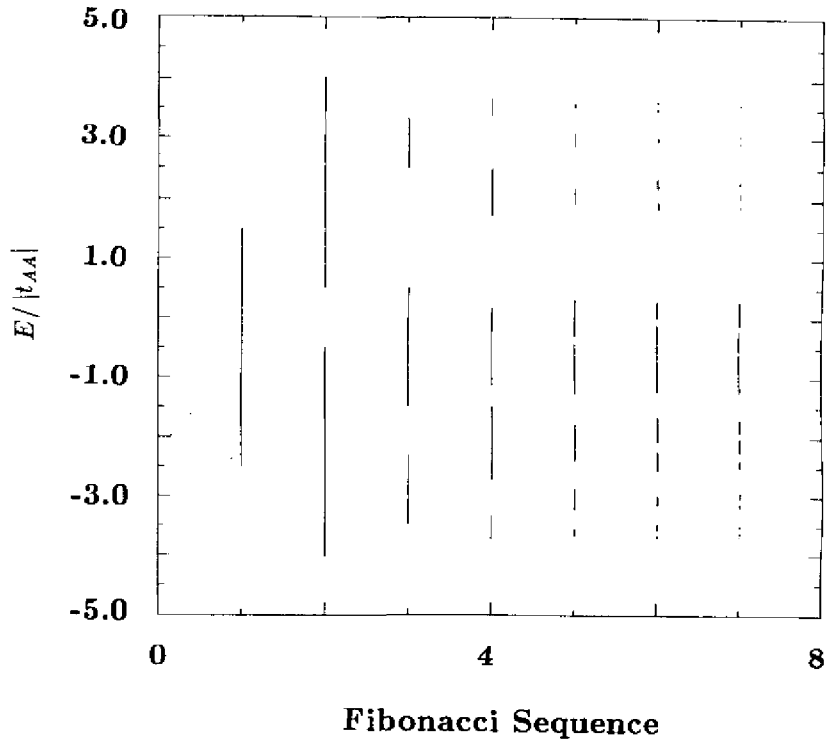

Fig.2

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