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LETTER TO THE EDITOR

Bloch-like states in a 1D Fibonacci chain

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Abstract. Certain types of wavefunctions with quasiperiodic amplitudes, which arise when blocks of two kinds of atoms are repeated in a Fibonacci sequence, are shown to have the same signature as the Bloch wavefunctions in terms of generalised dimensions.

The one-dimensional (1D) tight-binding model on a Fibonacci chain has been studied extensively as a model 1D quasicrystal [1]. Most attention has been paid to the study of the spectral properties [2, 3]. Much less attention has been paid to the study of the wavefunctions of the model [4, 5]. However, it is known that the wavefunctions are critical, corresponding to the singular continuous nature of the spectrum, although no rigorous proof exists [6]. In contrast, the Bloch states correspond to the absolutely continuous spectrum. Recently we discovered the existence of some wavefunctions at specific energies which behave much like the extended wavefunctions when blocks of atoms were repeated quasiperiodically [7]. Such wavefunctions have been seen in other systems [8]. The amplitude of these wavefunctions, though quasiperiodic, nearly repeats and hence the wavefunctions have the appearance of extended states. Recent studies of the wavefunctions show that there are two types of wavefunctions [4, 5], namely the self-similar wavefunctions at the band edges having a multifractal [9] nature and the chaotic wavefunctions which exhibit no particular scaling properties. Since other wavefunctions for this system are critical (mostly chaotic, corresponding to the chaotic but bounded trajectories of the trace map [10]), we should expect a crossover from the extended to the chaotic states. We have studied this crossover behaviour [4] using multifractal analysis. While characterising these wavefunctions we found [4] that even for a very large system size (~100000) these wavefunctions show an apparent multifractal nature, while the conventional Bloch states should have all the generalised dimensions $D(q) = 1$ for all q. Thus it is necessary to prove that these states have the same type of signature as the Bloch wavefunctions.

Consider the tight-binding Hamiltonian defined on a Fibonacci lattice by

$$E\psi_n = t_{n,n+1}\psi_{n+1} + t_{n,n-1}\psi_{n-1} + \varepsilon_n\psi_n. \qquad (1)$$

Here the site energies $\varepsilon_n = \varepsilon_A$ or ε_B appear in the Fibonacci sequence. For the sake of simplicity we choose the hopping integrals $t_{n,n+1} = t$. We have recently shown [7] that when blocks of atoms A and B of sizes N (>1) and M (>1), respectively, are repeated in a Fibonacci sequence then there exist some energies E_{ex} for which the wavefunctions behave like extended states. These energies are solutions of the matrix equation

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$\mathbf{T}_A^N = \pm\mathbf{I}$ or $\mathbf{T}_B^M = \pm\mathbf{I}$. Here $\mathbf{T}_A$ and $\mathbf{T}_B$ are the transfer matrices corresponding to the sites A and B, and $\mathbf{I}$ is the unit matrix. The maximum number of such states is $N + M - 2$. At these energies the invariant I of the trace map [1]

$$I = X_r^2 + X_{r-1}^2 + X_{r-2}^2 - 2X_rX_{r-1}X_{r-2} - 1$$

vanishes. Here $X_r = (\mathrm{Tr}\,\mathbf{M}_r)/2$ is the trace of the transfer matrix $\mathbf{M}_r$ of r Fibonacci blocks of atoms. For the sake of concreteness, we consider the case when $N = M = 2$. For this case, $E_{ex} = \pm w/2$, where $w = -\varepsilon_A = \varepsilon_B$. For $E = w/2$, we have

$$\mathbf{T}_A = \begin{pmatrix} -w/|t| & -1 \\ 1 & 0 \end{pmatrix} \qquad \mathbf{T}_B = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{2}$$

The wavefunction at a site $s = 2p + 2k$ with $2p$ A sites and $2k$ B sites is given by

$$\begin{pmatrix} \psi_{s+1} \\ \psi_s \end{pmatrix} = (-1)^k[\mathbf{T}_A]^{2p}\begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = (-1)^k\mathbf{S}\Lambda^{2p}\mathbf{S}^{-1}\begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} \tag{3}$$

where $\mathbf{S}$ diagonalises $\mathbf{T}_A$. Choosing $w = 2|t|\cos\theta$, we see that when p is an integer and $2\pi/\theta = p$, $\psi_{n\pm p} = \psi_n$ for p A sites and hence the wavefunction is periodic in p and therefore quasiperiodic in s. For other irrational values of p, $\psi_n \neq \psi_{n\pm p}$ for any p. Yet the envelope of the wavefunction looks very much like an extended state [4, 7]. Choosing $\psi_0 = \psi_1 = 1$, we obtain from (3)

$$\psi_s = [\sin(4p+1)\theta/2]/(\sin\theta/2) \qquad \text{even A sites} \tag{4a}$$

$$\psi_{s-1} = -[\sin(4p-1)\theta/2]/(\sin\theta/2) \qquad \text{odd A sites.} \tag{4b}$$

At this point it is worthwhile commenting on the usefulness of the method of finding the extended states in any quasiperiodic system. Consider the example A → ABBB, B → A [8]. This substitution rule satisfies the sequence $S_n = S_{n-1}S_{n-2}^3$ with the transfer matrices obeying the recursion relation $\mathbf{T}_n = \mathbf{T}_{n-2}^3\mathbf{T}_{n-1}$. The numbers of A atoms and B atoms are in the ratio $(1+\sqrt{13})/6$ and we note that the B atoms always appear in threes. Thus we can find the energies E_{ex} by demanding $\mathbf{T}_B^3 = \pm\mathbf{I}$. This gives $E - \varepsilon_B = \pm t$ with $|(\varepsilon_B - \varepsilon_A \pm t)/t| < 2$. For all these allowed values of the parameters we get two extended states. A plot of one such wavefunction for $\varepsilon_B = -\varepsilon_A = -0.49$ and with $E_{ex} = 0.51$ is shown in figure 1.An alternative way of locating the extended states is to calculate the energies at which the invariant I of the trace map vanishes. However, it is often not possible to calculate I for all types of quasiperiodic sequences. Where it is possible, obtaining solutions of $I(E) = 0$ is not easy when blocks of atoms are large. Thus the method presented here is simple and straightforward.

Using multifractal analysis we show that these wavefunctions have the same signature as the extended states. Below we briefly recapitulate the multifractal method and study the scaling behaviour of the wavefunction given by (4). We first normalise the wavefunction in the given interval and then choose the probability measure P_i to be $|\psi_i|^2$ with a uniform Lebesgue measure $l = 1/F_r$. The scaling of the probability measure is taken as $P_i \sim l^\alpha$, where α has a spectrum of singularities given by $f(\alpha)$ for a multifractal wavefunction. Specifying $f(\alpha)$ completely characterises the wavefunction. For the Bloch wavefunctions $f(\alpha) = \alpha = 1$. These quantities are calculated by computing $\chi(q) = \Sigma_i P_i^q$, which scales as $l^{\tau(q)}$. Then $\tau(q)$ is related to $f(\alpha)$ through

$$\tau(q) = D(q)(q-1) \qquad \partial\tau/\partial q = \alpha \qquad \tau = \alpha q - f(\alpha) \tag{5}$$

where the $D(q)$ are the generalised dimensions.

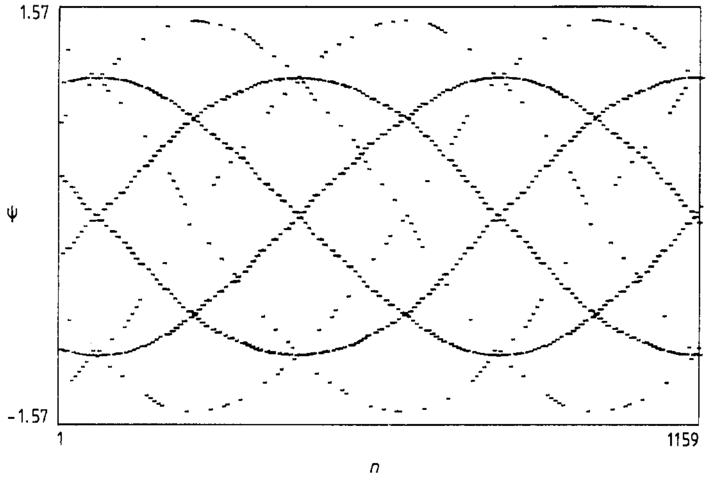

Figure 1. A plot of the extended wavefunction ψ_n versus n for $\varepsilon_B = -\varepsilon_A = 0.49$ and $E = 0.51$ with $\psi_0 = 1$ and $\psi_1 = 0.3$.

In order to calculate the normalised wavefunctions, it is necessary to consider the nature of the quasiperiodic sub-sequences of the A and B atoms which had been discussed in the context of diffusion on a Fibonacci chain [11]. We note that there are three types of sites namely α, β and γ appearing in the sequence $\beta\gamma\alpha\beta\gamma\beta\gamma\alpha\beta\gamma\alpha\beta\gamma$ . . . with a frequency of occurrence $\omega^{-1}:1:1$, where $\omega = (\sqrt{5}+1)/2$ is the golden mean. The sites α, β and γ occur between L and L, L and S, and S and L. The A blocks occupy the α and γ sites, and the B blocks occupy the β sites. Furthermore, the β sites always precede the γ sites and thus $|\psi|$ at the β sites have the same value as at the odd γ sites. Therefore, it is sufficient to consider the sum over the α and the γ sites for evaluating the normalisation constant. Let $s = 2F_{r+1}$; then there are $2F_{r-2}$ A atoms at the α sites, $2F_{r-1}$ A atoms at the γ sites and $2F_{r-1}$ B atoms at the β sites. Thus we have

$$\bar{A}\sum_{p}|\psi_s(k,q)|^2 = \bar{A}\left(\sum_{p_\gamma}|\psi_s(k,p)^2| + \sum_{p_\alpha}|\psi_s(k,p)|^2 + 2\sum_{p_\gamma(\mathrm{odd})}|\psi_s(k,p)|^2\right) = 1. \tag{6}$$

The last term represents the sum corresponding to the β sites due to the fact that $|\psi|$ at the β has the same value as at the odd γ sites. These sums can be performed by using the projection technique [2, 3]. Although three different sites are involved, we are interested in calculating the sum over the A sites and hence it is adequate to use slits corresponding to the α–γ sub-sequence. Consider evaluating the first term (apart from a factor of $\sin^2\theta/2$). This can be written as

$$\sum_{p_\gamma(\mathrm{even})}^{F_{r-1}} \{2 - \exp[-\mathrm{i}(4p+1)\theta] - \exp[\mathrm{i}(4p+1)\theta]\}. \tag{7}$$

In the limit of large r, the last two terms can be obtained by the projection method along the lines given in [2, 3]. For instance we get

$$\sum_{p_\gamma(\mathrm{even})} \exp(\pm\mathrm{i}4p\theta) = \sum_{n,m} [\exp(\mathrm{i}\varphi_{nm})(\sin\varphi_{nm})\,\delta(4\theta \pm \kappa_{nm})]/\omega\varphi_{nm}. \tag{8}$$

Here $\varphi_{nm} = \pi(n-m)/\omega$ and $\kappa_{nm} = 2\pi(n+n\omega)/(N+M\omega)$ is the wavevector for the

Fibonacci lattice ($N = M = 2$). In the limit of large r it is clear that the δ function does not contribute since both θ and κ_{nm} are in general two different irrational numbers. Thus the first term gives the dominant contribution equal to $2F_{r-1}$. It is easy to show that the odd terms have an equal contribution. In a similar way, the contribution from the odd and even α sites can be shown to be $4F_{r-2}$. An equal contribution arises for the β sites. Thus one gets

$$\bar{A} \sum_{s} |\psi(k,p)^2| \simeq \bar{A} F_{r+1}/\sin^2(\theta/2) = 1. \tag{9}$$

Thus the normalised wavefunctions Ψ in the large r limit are

$$\Psi_s(k,p) = \sin(4p+1)\theta/F_{r+1} \qquad \text{even A sites} \tag{10a}$$

$$\Psi_{s-1}(k,p) = -\sin(4p-1)\theta/F_{r+1} \qquad \text{odd A sites.} \tag{10b}$$

Following the above lines we can calculate $\chi(q)$ by again splitting the sum into three parts as above. Consider one such sum. It is easy to see that the leading term is

$$\sum_{p_\gamma} \{2 - \exp[-\mathrm{i}(4p+1)\theta] - \exp[\mathrm{i}(4p+1)\theta]\}^q \sim 2^q F_{r-1}.$$

An equal contribution arises from the β sites. The sum corresponding to α sites is $2^q F_{r-2}$. (In addition, there is a term arising from equal powers of the exponentials in the expansion which only changes the contribution up to a multiplicative factor and is therefore unimportant.) Thus, $\chi(q) = [2F_{r+1}]^{1-q}$ and hence we find

$$\tau(q) \sim q - 1 \qquad f(\alpha) = \alpha = 1. \tag{11}$$

This is what is expected for a conventional extended wavefunction. When N and M are greater than two, it is possible to perform a similar calculation, though much more tedious. In such an instance one needs to obtain the N and M wavefunctions within the A block and the B block by supplying an appropriate number of transfer matrices of A or B. When the sizes of these blocks are large, it is clear that the number of such states grows linearly with the sizes of the blocks and in this limit within each block the profile of the wavefunction would be like that of a periodic system. A few comments may be in order on the slow numerical convergence $\tau(q)$ as a function of the size of the system. Let $\chi_r(q)$ and $\tau_r(q)$ represent the values of $\chi(q)$ and τ corresponding to a Fibonacci chain length F_r. Then

$$\chi_r(q) \sim l^{\tau_r(q)} \sim F_r^{-\tau_r r(q)} \sim \omega^{-r\tau_r(q)}.$$

$\tau_r(q) \to 1$ as $r \to \infty$; thus $\tau_r(q) \sim 1/r$ and hence the slow convergence.

The effect of the finite size of the system, the slow convergence and the scaling law are well illustrated by considering a plot of $\tau_r(q)$ as a function of q for various lengths of the chain (calculated numerically by using $l = F_r^{-1}$). Figure 2 contains a plot of $\tau_r(q)$ for $r = 19$ to 23 and the extrapolated $\tau_\infty(q)$ which is linear in q. The inset contains the scaling of $\tau_r(q)$ as a function of r, for $q = 10$. A few comments may be in order. First, it must be pointed out that the limiting behaviour $\tau_\infty(q) \propto q - 1$ can be obtained in the following way. Let the chain of length $2F_r$ be divided into m segments of length l. Define

$$P_k = \sum_{i=(k-1)l}^{kl} |\psi_i|^2 \qquad \chi(q) = \sum_{k=1}^{m} P_k^q .$$

When l is chosen to be of the order of a few blocks one finds $\tau(q) \propto q - 1$. The extent of l represents the length over which the wavefunction exhibits a correlation below which

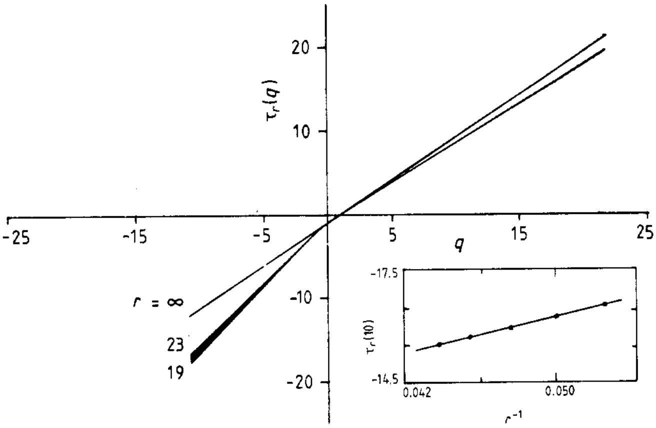

Figure 2. Plot of numerically calculated $\tau_r(q)$ versus r for $r = 19$ to 23 and the extrapolated $\tau_\infty(q)$. Inset: $\tau_r(q)$ scaling as r^{-1}, for $q = 10$.

one finds a change in the curvature of $\tau(q)$ against q. Second, in the case of the Thue–Morse sequence one may be led to think that convergence is non-monotonic, but one finds in reality several independent sequences which converge to the same limiting value. In this case the convergence is more rapid. For instance for $r = 14$, $S_r = 75316$, the change in curvature is hardly noticeable.

In conclusion we have demonstrated that the quasiperiodic wavefunctions corresponding to certain energies E_{cx} have the same signature as conventional Bloch states.

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References

[1] Kohmoto M, Kadanoff L P and Tang C 1983 *Phys. Rev. Lett.* **50** 1870
Ostlund S, Pandit R, Rand D, Schellnhuber H J and Siggia E 1983 *Phys. Rev. Lett.* **50** 1873
[2] Nori F and Rodriguez P 1986 *Phys. Rev.* B **34** 2207
Zia R K P and Dallas W 1985 *J. Phys. A: Math. Gen.* **18** L341
[3] Valsakumar M C and Ananthakrishna G 1987 *J. Phys. C: Solid State Phys.* **20** 9
[4] Ananthakrishna G and Kumar V 1989 submitted
[5] Fujiwara T, Kohmoto M and Tokihiro T 1989 *ISSP, University of Tokyo, Technical Report*
[6] Delyon F and Petritis D 1986 *Commun. Math.* **103** 441
[7] Kumar V and Ananthakrishna G 1987 *Phys. Rev. Lett.* **59** 1476
Ananthakrishna G and Kumar V 1988 *Phys. Rev. Lett.* **60** 1586
See also Ananthakrishna G 1989 *Proc. Int. Conf. on Modulated Structures, Polytypes and Quasicrystals (Varanasi, India, December 1988)*
[8] Severin M and Riklund R 1989 *Phys. Rev.* B **39** 10362
[9] Henstschel H G E and Procaccia I 1983 *Physica* D **8** 835
Halsey T C, Jensen M H, Kadanoff L P, Procaccia I and Shraiman B I 1986 *Phys. Rev.* A **33** 1141
[10] Kohmoto M, Sutherland B and Tang C 1987 *Phys. Rev.* A **35** 1020
[11] Ananthakrishna G and Balasubramanian T 1988 *Bull. Mater. Sci.* **10** 77