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LETTER TO THE EDITOR

Scaling and eigenstates for a class of one-dimensional quasiperiodic lattices

Godfrey Gumbs and M K Ali

Department of Physics, University of Lethbridge, Lethbridge, Alberta, T1K 3M4 Canada

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Abstract. Numerical and analytical calculations of the electronic properties of a one-dimensional quasiperiodic lattice are presented. The lattice consists of two types of bonds A and B whose distribution follows the recursion formula $S_{l+1} = S_{l-1}^m S_l^n$ where $m, n = 1, 2, 3, \ldots$ and S_l is a building block sequence for $l \geq 2$. An exact evaluation of the wavefunction yields the scaling for several pairs of values of m and n. Numerical calculations of the wavefunction and the resistance reveal a rich self-similar structure as well as localisation for one of the quasiperiodic sequences studied.

In this letter, we report the results of calculations of the electronic eigenstates of the tight-binding model [1, 2]

$$\begin{pmatrix} \psi_{l+1} \\ \psi_l \end{pmatrix} = M(T_{l+1}, T_l) \begin{pmatrix} \psi_l \\ \psi_{l-1} \end{pmatrix} \tag{1}$$

where ψ_l denotes the wavefunction for a state with energy E at the lth lattice site and $\{T_l\}$ is a quasiperiodic sequence with two kinds of hopping matrix elements T_A and T_B. $M(T_i, T_j)$ is a transfer matrix given by

$$M(T_i, T_j) \equiv \begin{pmatrix} E/T_i & -T_j/T_i \\ 1 & 0 \end{pmatrix}. \tag{2}$$

Successive applications of the transfer matrices give the wavefunction at arbitrary sites. The main problem is therefore to calculate the product of matrices

$$M(l) = M(T_{l+1}, T_l) M(T_l, T_{l-1}), \ldots, M(T_2, T_1). \tag{3}$$

The quasiperiodic lattices we investigate here are, in some sense, a generalisation of the Fibonacci lattice. When F_l is a generalised Fibonacci number given recursively by $F_{l+1} = mF_{l-1} + nF_l$ where m and n are positive integers and $F_0 = F_1 = 1$, $M(l)$ can be obtained recursively. With $M_l = M(F_l)$, we obtain

$$M_{l+1} = M_{l-1}^m M_l^n \tag{4}$$

where $M_1 = M(T_A, T_A)$ and $M_2 = M(T_A, T_B) M(T_B, T_A)$. The recursion relation in (4) is extremely useful in carrying out numerical calculations. In addition, this recursion formula defines a non-linear dynamical map for which we could apply the concept of dynamical systems. Defining $x_l = \frac{1}{2} \operatorname{Tr} M_l$, where $\operatorname{Tr}(\ldots)$ denotes the trace of a matrix, we have explicitly calculated the recursion relation for x_l for four pairs of values of m and n. These are now given.

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For $m=1$ and $n=1$, the ratio of successive Fibonacci numbers F_{l+1}/F_l tends to the golden mean $\sigma_G \equiv (5^{1/2}+1)/2$ in the limit $l \to \infty$. The map for the trace is well known and is given by $x_{l+1} = 2x_l x_{l-1} - x_{l-2}$.

For $m=1$ and $n=2$, the ratio of successive Fibonacci numbers tends to the silver mean $\sigma_S = 2^{1/2}+1$. The dynamical map is obtained by taking the trace of the equation

$$M_{l+1} + M_{l-1} = M_{l-1} M_l (M_l + M_l^{-1}). \tag{5}$$

Defining $t_l \equiv \mathrm{Tr}(M_{l-2}M_{l-1})/4$, we obtain the pair of equations

$$x_{l+1} = 4x_l t_{l+1} - x_{l-1} \tag{6a}$$

$$t_{l+1} = x_{l-1}x_l - t_l \tag{6b}$$

subject to the initial conditions $t_2 = x_1 T_A/(2T_B)$. Whenever the recursion relations (6) are satisfied, the quantity

$$I_S = x_l^2 + x_{l+1}^2 + 4t_{l+2}^2 - 4x_l x_{l+1} t_{l+2} - 1 \tag{6c}$$

is unchanged by successive iterations.

For $m=1$ and $n=3$, the ratio of successive Fibonacci numbers tends to the bronze mean $\sigma_B = (13^{1/2}+3)/2$. In this case, the dynamical map is obtained by taking the trace of the equation

$$M_{l+1} + (M_{l-1}M_l^{-1} + M_{l-2}) - M_{l-2} = M_{l-1}M_l(M_l^2 + M_l^{-2}). \tag{7}$$

This yields

$$x_{l+1} = (4x_l^2 - 1)g_{l+1} - 2x_{l-1}x_l \tag{8a}$$

$$g_{l+1} = 2x_{l-1}(x_l - g_l) + x_{l-2} \tag{8b}$$

where $g_l \equiv \mathrm{Tr}(M_{l-2}M_{l-1})/2$. The map in (8) has a constant independent of l given by

$$I_B = x_{l-1}^2 + x_l^2 + g_{l+1}^2 - 2x_{l-1}x_l g_{l+1} - 1. \tag{8c}$$

When $m=2$ and $n=1$, the trace map takes the form†

$$x_{l+1} = (4x_{l-1}^2 - 2)x_l + \gamma \tag{9}$$

where γ is independent of l and given by $\gamma = x_2 - Ex_1/T_B$. In this case, the ratio of successive terms F_{l+1}/F_l tends to the copper mean $\sigma_C = 2$.

We consider the electron wavefunction at the centre of the band, $E=0$. A detailed study of the eigenfunction and allowed band energy for the Fibonacci lattice with the golden mean has been presented in the literature [1, 3]. For the quasiperiodic lattices with the silver, bronze and copper means, the magnitude of the wavefunction is plotted in figures 1–3, as a function of the lattice site number along the quasiperiodic lattice for $E=0$ and $R \equiv T_B/T_A$. While the wavefunction in figures 1 and 2 are self-similar, like the wavefunction for the Fibonacci lattice with the golden mean, and are neither

† Equation (9) is obtained by writing the recursion relation for the matrices in (4) for $m=2$ and $n=1$ as

$$M_{l+1} + M_{l-1}^{-2} M_l = (M_{l-1}^2 + M_{l-1}^{-2}) M_l$$

and taking the trace of this equation. This gives the trace map in (9) with the last term defined by

$$\gamma \equiv -\tfrac{1}{2}\,\mathrm{Tr}(M_{l-1}^{-2}M_l).$$

Whenever the recursion relation for the transfer matrices is satisfied this quantity is independent of l. Thus γ is determined from the initial conditions and is an invariant for the map with the copper mean.

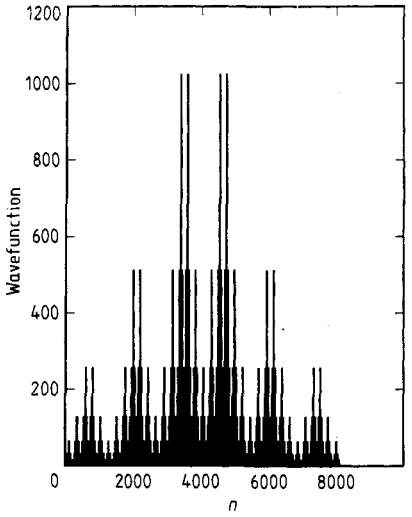

Figure 1. The electronic wavefunction at $E=0$ for $R=T_B/T_A=2.0$. The figure is a plot of the magnitude of the wavefunction $|\psi_n|$ against the site number n along the quasiperiodic direction for the lattice with the silver mean. We choose $\psi_0=0$ and $\psi_1=1$.

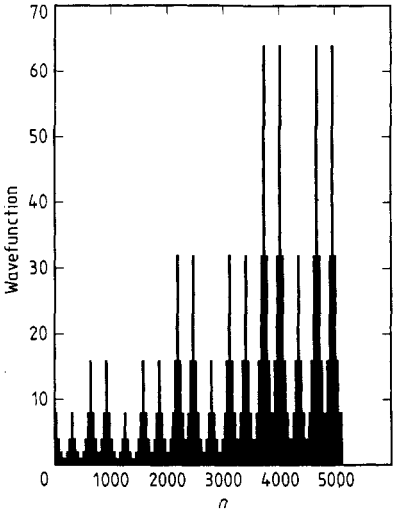

Figure 2. Same as figure 1 for the wavefunction at the centre of the band $E=0$ for the lattice with the bronze mean.

extended nor localised in a standard way, the lattice with the copper mean is indeed localised. This result is one of the main results of this letter since this type of localisation has never been exhibited for a one-dimensional quasiperiodic lattice structure. The series of peaks in figures 1 and 2 have values which increase as a power of R. This power law behaviour could be calculated in the way adopted by Kohmoto and Banavar [3] for the Fibonacci lattice with the golden mean. For the silver mean, consider the transfer matrix

$$M(N)=M_3M_5M_7M_9,\ldots,M_{4p+1}=(-1)^p\begin{pmatrix}1/R^{2p} & 0\\ 0 & R^{2p}\end{pmatrix} \tag{10}$$

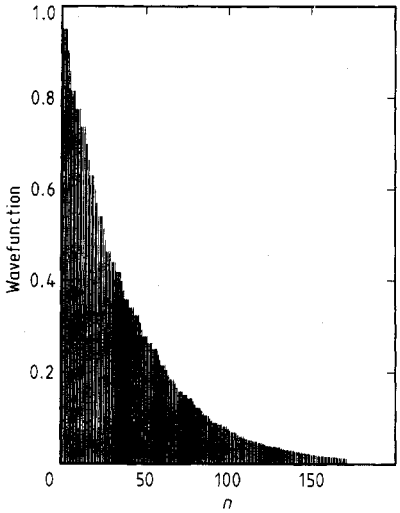

Figure 3. Same as figure 1 for the lattice with the copper mean except that $R = 0.95$.

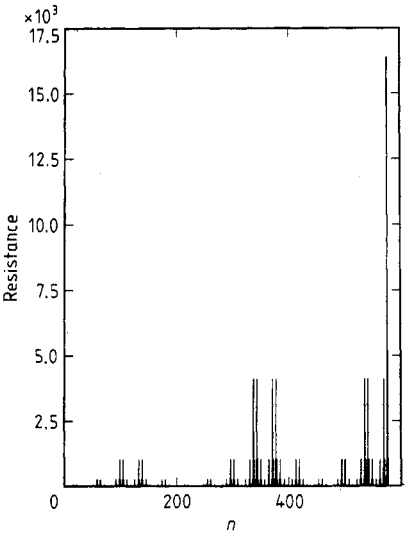

Figure 4. The resistance against site number for $E = 0$ corresponding to the Fibonacci lattice with the silver mean.

where p is an integer and

$$N = F_3 + F_5 + F_7 + F_9 + \ldots + F_{4p+1} \tag{11}$$

($N = 48$, 1680, 57 120, ...). Equation (10) gives a series of peaks

$$\psi_N = (-1)^p R^{2p} \psi_0. \tag{12}$$

For large values of N, it is a simple matter to show that (12) yields the power law behaviour

$$|\psi_N| \sim N^{\beta_S} \psi_0 \tag{13}$$

where $\beta_S \equiv \ln R / \ln \sigma_S^2$ is the scaling exponent for the lattice with the silver mean. The

wavefunction at $E = 0$ for the Fibonacci lattice with the bronze mean could be calculated exactly at the lattice sites $N = F_3 + F_6 + \ldots + F_{3\times 2p}$. For large values of N, this wavefunction has a power law behaviour with the exponent in (13) replaced by $\beta_B \equiv 2 \ln R / 3 \ln \sigma_B$. For the lattice with the copper mean, the wavefunction for the special energy $E = 0$ could be obtained by a simple formula at the lattice sites with a Fibonacci number. Numerical calculations show that the plot of wavefunction at $E = 0$ against the lattice site along the chain is monotonic. This is shown in figure 3. Thus the lattice with the copper mean is the only one of the cases studied so far which shows this type of behaviour for the wavefunction.

We now turn to the resistance of the tight-binding model in (1) for a linear chain with N lattice sites. This quantity, defined as the ratio between total reflection and transmission coefficients, is given by [4-6]

$$\rho = \frac{1}{4 \sin^2 k} \{ \| M_N \|^2 + 2(\cos k)(M_N^{11} - M_N^{22})(M_N^{12} - M_N^{21}) - 4(\cos^2 k) M_N^{12} M_N^{21} - 2 \} \qquad (14)$$

where $\| M_N \|^2$ is the sum of the squares of the elements of the 2×2 matrix $M_N \equiv M(N)$ defined in (3). We also define the energy in terms of the wavevector k by $E = 2T_0 \cos k$, where the hopping matrix elements are equal to a constant T_0 outside the disordered segment $1 \leq l \leq N$. Following the arguments above for the wavefunction, the power law behaviour and scaling of the ρ could be obtained for the lattice with the silver and bronze means as derived in [6] for the golden mean. In figure 4, $R = 2.0$.

The non-periodicity of the lattice with the copper mean is obviously strong enough to cause the wavefunction to decay as a function of distance from the origin. However, the localisation is not as strong as the localisation in the one-dimensional disordered system which was conjectured by Mott and Twose [7] and proven by others [8, 9]. For this kind of (Anderson) localisation, the envelope of the amplitude of the wavefunction decays exponentially from some point in space (see the review of Lee and Ramakrishnan [10] and the very clear presentation by Tong [11] for localisation in a one-dimensional model having disorder). Subsequently, we conclude that the class of lattices given recursively by (4) could be divided up into two subclasses depending on the localisation properties of the wavefunction. This separation of the lattices was also evident by studying the dynamical maps for the traces of the matrices [12]. Additional numerical and analytical calculations dealing with ternary strings will be published elsewhere.

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References

[1] Kohmoto, M, Sutherland B and Tang C 1987 *Phys. Rev.* B **35** 1020
[2] Kohmoto M, Sutherland B and Iguchi K 1987 *Phys. Rev. Lett.* **58** 2436
[3] Kohmoto M and Banavar J 1986 *Phys. Rev.* B **34** 563
[4] Landauer R 1970 *Phil. Mag.* **21** 863
[5] Stone A D, Joannopulos J D and Chadi D J 1981 *Phys. Rev.* B **24** 5583
[6] Schneider T, Politi A and Würtz D 1987 *Z. Phys.* B **66** 469
[7] Mott N F and Twose W D 1961 *Adv. Phys.* **10** 107
[8] Borland R E 1963 *Proc. R. Soc.* A **274** 529
[9] Hori J and Minami S 1968 *Localized Excitations in Solids* ed R F Wallis (New York: Plenum) p 611
[10] Lee P A and Ramakrishnan T V 1985 *Rev. Mod. Phys.* **57** 287
[11] Tong B Y 1970 *Phys. Rev.* A **1** 52
[12] Gumbs G and Ali M K 1988 *Phys. Rev. Lett.* **60** 1081