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1986 J. Phys. C: Solid State Phys. 19 L823

(http://iopscience.iop.org/0022-3719/19/34/005)

J. Phys. C: Solid State Phys. **19** (1986) L823–L827. Printed in Great Britain

LETTER TO THE EDITOR

Electronic structure of one-dimensional quasi-crystals

Hong-ru Ma†, Yun Xu† and Chien-hua Tsai‡§

† Institute of Condensed Matter Physics, Jiao-Tong University, Shanghai, People's Republic of China

‡ Department of Theoretical Physics, School of Physics, University of New South Wales, PO Box 1, Kensington, New South Wales 2033, Australia

Received 27 August 1986

Abstract. The electronic structure of a one-dimensional quasi-crystal in the form of a Fibonacci sequence is computed in terms of a tight-binding model.

The discovery of icosahedral symmetry in quenched $Al_{0.86}Mn_{0.14}$ (Shechtman *et al* 1984) has stimulated great interest in the study of quasi-crystals. However, only a few studies (Kohmoto and Sutherland 1986, Lu *et al* 1986, Odagaki and Nguyen 1986) concerning the basic electron and phonon structures of quasi-crystals have appeared, and this was very recently. We report here results of a computation of the electron structure of one-dimensional quasi-crystals in the form of a Fibonacci sequence. Superlattice structures have been observed in quenched Al–Si–Mn quasi-crystals (Chen and Chen 1986). However, quasi-superlattices with superstructures modulated quasi-periodically may be more interesting physically, in view of the possibility of artificial control of the samples under observation. We expect our results to be of significance for quasi-superlattices.

We postulate the following one-dimensional tight-binding Hamiltonian:

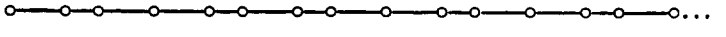

Figure 1. A schematic diagram of a one-dimensional Fibonacci quasi-crystal.

$$\mathbf{H} = \sum_i |i\rangle \varepsilon_i \langle i| + \sum_{i,j} |i\rangle T_{ij} \langle j| \tag{1}$$

where, in accordance with a Fibonacci sequence (see figure 1), we consider

$$\varepsilon_i = \begin{cases} \varepsilon_1 & \text{when site } i \text{ is connected to both nearest neighbours by long bonds} \\ \varepsilon_2 & \text{otherwise} \end{cases} \tag{2}$$

§ On sabbatical leave from the Department of Physics, Jiao-Tong University, Shanghai, People's Republic of China.

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and

$$T_{ij} = \begin{cases} T_1 & \text{when } j = i \pm 1 \text{ and sites } i \text{ and } j \text{ are connected by a long bond} \\ T_2 & \text{when } j = i \pm 1 \text{ and sites } i \text{ and } j \text{ are connected by a short bond} \\ 0 & \text{otherwise.} \end{cases} \tag{3}$$

In the site representation, **H** is tri-diagonal. In order to find the distribution of its eigenvalues or, equivalently, the electronic density of states (DOS), we adopt the negative-eigenvalue theory of Dean (1972). Let $\eta(E)$ be the number of negative eigenvalues of the matrix $\mathbf{H} - E\mathbf{I}$; then the number of eigenvalues per unit energy range is given by

$$N(E) = (\eta(E + \Delta E) - \eta(E))/\Delta E \tag{4}$$

whereas the DOS is

$$\rho(E) = N(E)/\mathcal{N} \tag{5}$$

where $\mathcal{N}$ is the rank of the matrix. Dean (1972) has proved that

$$\eta(E) = \sum_i \eta_i(E) \tag{6}$$

where $\eta_i(E)$ can be evaluated in the following way: form the sequence

$$\begin{aligned} n_1 &= \varepsilon_1 - E \\ n_i &= \varepsilon_i - E - T_{i,i-1}T_{i-1,i}/n_{i-1} \end{aligned} \tag{7}$$

then

$$\eta_i(E) = \begin{cases} 0 & \text{when } n_i > 0 \\ 1 & \text{when } n_i < 0. \end{cases} \tag{8}$$

With $\mathcal{N} = 10000$, the DOS obtained in the above-explained manner are given in figures 2 to 4 for different choices of parameters. Figure 2 corresponds to the case of a periodic one-dimensional crystal. In order to make sure that 'noises' arising from the finite length of the chain do not affect the DOS strongly, we performed computations in

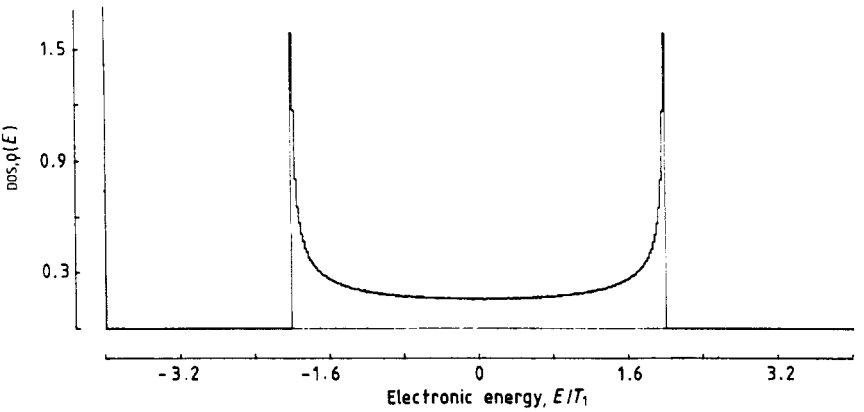

Figure 2. The electronic DOS of a one-dimensional periodic crystal. $\varepsilon_1 = \varepsilon_2 = 0$. $T_1 = T_2 = 1$.

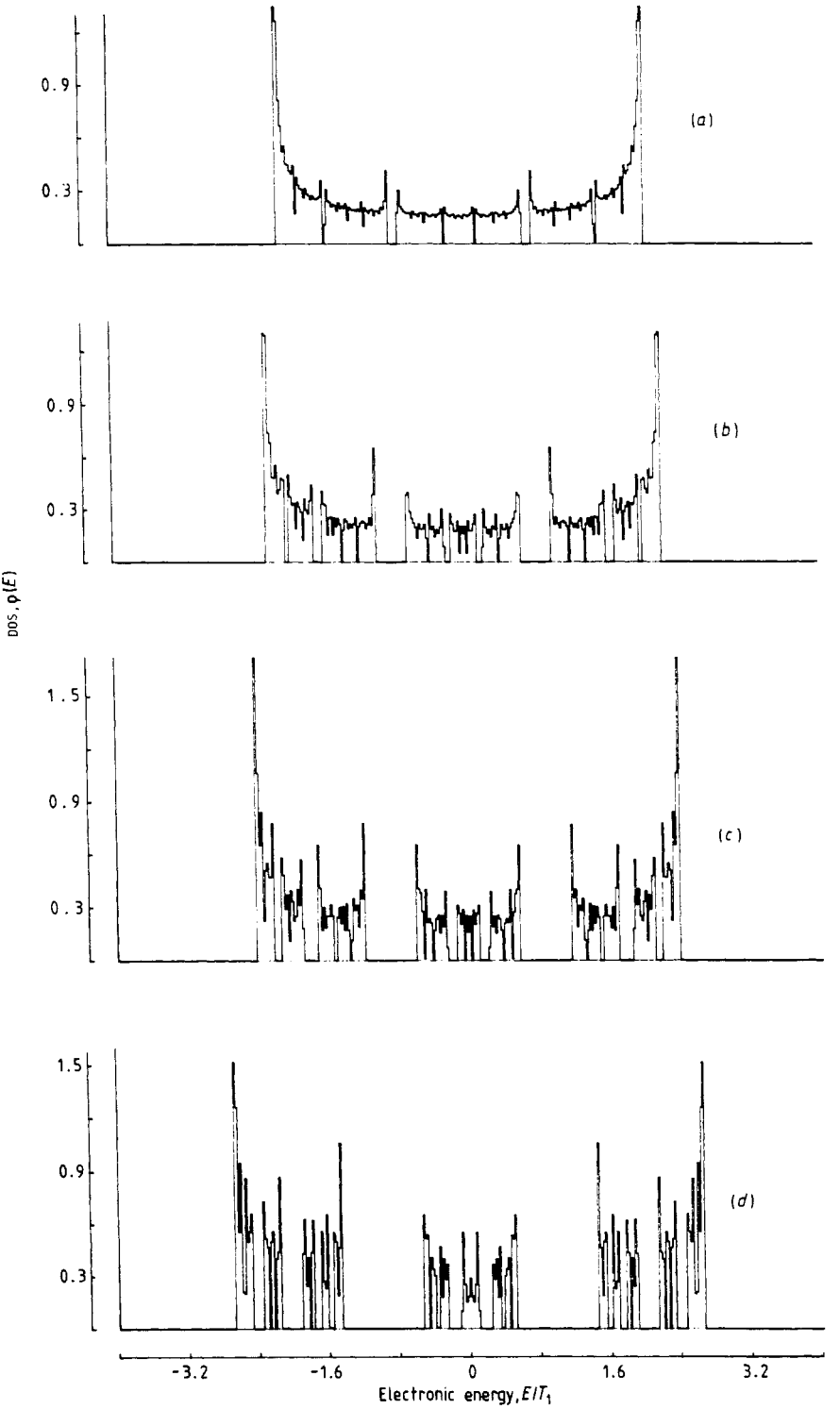

Figure 3. The electronic DOS of a one-dimensional Fibonacci quasi-crystal for the symmetrical case: $\varepsilon_1 = \varepsilon_2 = 0$. $T_1 = 1$. $T_2 =$ (*a*) 1.1, (*b*) 1.3, (*c*) 1.5, (*d*) 1.8.

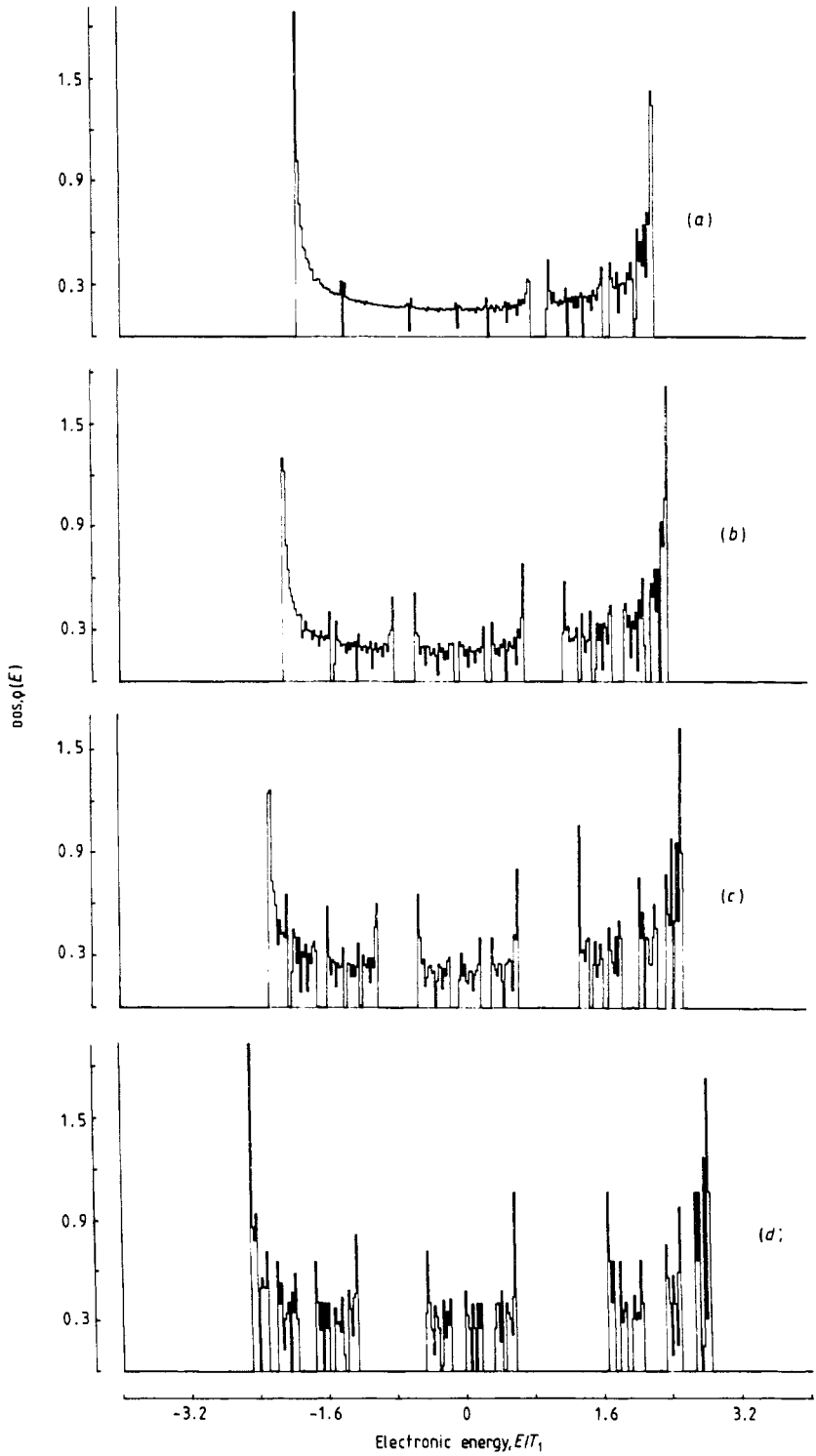

Figure 4. The electronic DOS of a one-dimensional Fibonacci quasi-crystal for the asymmetrical case: $\varepsilon_1 = 0$, $\varepsilon_2 = 0.2$. T_1, T_2 are as for figure 3.

this case with periodic boundary conditions too, and the results showed no discernible difference from the profile in figure 2. Figure 3 displays the electronic DOS for $\varepsilon_1 = \varepsilon_2 = 0$, so DOS profiles are symmetrical with respect to the origin of the energy scale. Figure 4 is for the asymmetrical case $\varepsilon_1 = 0$, $\varepsilon_2 = 0.2$. In both cases, the increasing departure from the profile of periodic structures (figure 2) with increasing difference between values of T_1 and T_2 is obvious. Moreover, the electronic energy spectrum consists of a large number of narrow bands with rich microstructures, so the electronic states are presumably localised as in the case of one-dimensional incommensurable systems (Dy and Ma 1982, Dy and Wang 1984).

One of the authors (Chien-hua Tsai) would like to acknowledge a grant from the Australian Research Grant Scheme. He would also like to acknowledge the hospitality of the University of New South Wales and of Professor D Neilson of the School of Physics and Dr B N Kaye of New College as well as helpful discussions with Professor K N R Taylor, Professor D Neilson and Dr G J Russell.

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