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The electronic density of states of an infinite one-dimensional Fibonacci chain

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Abstract. In this paper, we describe an analytical approach for studying the electronic density of states of an infinite one-dimensional Fibonacci chain using the on-site model. We have identified uniquely a set of short-range order parameters appropriate to the Fibonacci chain and used them in the theory based on the cluster–Bethe-lattice method which has been described elsewhere. We have found that both the local density of states and the average density of states exhibit a four-sub-band global structure and each sub-band further trifurcates following a hierarchy of splitting from one to three sub-bands until the gaps between them disappear. The positions of the various sub-bands and their widths are in good agreement with the numerical results of Liu and Riklund.

The discovery of the icosahedral symmetry in the metallic alloy Al–Mn by Schechtman and co-workers [1] has motivated extensive research in the understanding of the electronic properties of quasi-periodic systems, both in one dimension and higher dimensions [2–9]. A Fibonacci lattice is the one-dimensional (1D) version of the Penrose tiling [10] and the icosahedral quasi-crystals [11], which has become an interesting object of study in recent years. The study of such 1D quasi-periodic (QP) systems has become particularly relevant since the success of Merlin and co-workers [12] in growing a QP Fibonacci superlattice and carrying out x-ray and Raman scattering measurements on it.

Recently, there have been a number of studies of the vibrational and electronic spectrum of 1D QP systems. Two different kinds of model, namely, the transfer model and the on-site model, both based on the tight-binding Hamiltonian, have been introduced [2, 5] for studying the electron states of 1D QP systems. The energy spectra for these two models have been studied by several authors using both renormalisation group (RG) techniques [2, 3] and numerical methods [4, 5]. Of particular interest is the RG approach of Wurtz and co-workers [3], which handles the Schrödinger equation for the combined on-site and transfer model exactly. However, less attention has been paid to the electronic density of states (DOS) for a Fibonacci chain so far. Mookerjee and Singh [13] have studied the average DOS for the transfer model using the recursion method of Haydock and co-workers [14]. In this paper, we report a new analytical technique for obtaining the local density of states (LDOS) for an infinite Fibonacci chain described by the on-site model. In our method the accuracy of the LDOS can be made arbitrarily high without much escalation of computational effort. Both the LDOS and the averaged LDOS exhibit four-sub-band global structure and each sub-band in turn splits into three sub-bands in a hierarchical manner until the gaps between them vanish. The positions of

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these bands fit quite accurately with the numerical results of Liu and Riklund [5].

For our case we use the tight-binding Hamiltonian

$$H = \sum_{i=-\infty}^{\infty} \varepsilon_i |i\rangle\langle i| + \sum_{i=-\infty}^{\infty} t(|i\rangle\langle i+1| + |i\rangle\langle i-1|) \tag{1}$$

where the site energies ε_i can assume the values ε_A and ε_B, and they are distributed according to the Fibonacci sequence, and the nearest-neighbour hopping integral has a constant value t. The desired Fibonacci chain can be generated by the repeated application of the substitution rule $A \rightarrow AB$ and $B \rightarrow A$, taking A as the starting point. In this way, the first few generations are the segments A, AB, ABA, ABAAB . . . etc. We have studied both LDOS and the averaged LDOS for an infinite Fibonacci chain generated in this manner. As this system has no periodicity, the local environments vary from site to site but the lattice has a perfect long-range order as dictated by the Fibonacci sequence. Such systems are thus intermediate between crystalline solids and disordered alloys. A very useful technique for handling such problems is the cluster–Bethe-lattice method (CBLM) [15] which reproduces the connectivity of the lattice exactly in the 1D case. The essence of this method consists in isolating a finite cluster of atoms of the actual lattice around a specified central atom and replacing the rest of the infinite system by a suitable effective medium, so chosen as to reproduce the gross and large-scale features of the system. In this approach the accuracy of the results may be improved arbitrarily by increasing the cluster size, the effective medium playing a comparatively minor role in so far as the calculation of the LDOS is concerned [16]. We thus content ourselves by describing the effective medium in terms of the concentrations of the A and B atoms and by a set of short-range order (SRO) parameters that are appropriate to the Fibonacci chain. The details of this approach may be found in [17].

The ratio of the numbers of A and B atoms in the infinite chain is given by the Golden Ratio τ, which has the value $(1 + \sqrt{5})/2$, from which the concentrations x and y of the A and B atoms are seen to be $\tau/(1 + \tau)$ and $1/(1 + \tau)$ respectively. We describe the local environmental ordering using a set of SRO parameters in the manner of Falicov and Yndurain [18], by introducing the quantity $p_{A(B)}$, which represents the conditional probability that a given A (B) atom has an A (B) atom as its nearest neighbour. Similarly, we define the parameter $q_{A(B)}$ which is the conditional probability that an A (B) atom has a B (A) atom as its nearest neighbour. From the conservation of probabilities we have

$$p_A + q_A = p_B + q_B = 1. \tag{2}$$

Moreover, the fact that the number of bonds connecting dissimilar atoms may be found in two ways yields

$$xq_A = yq_B. \tag{3}$$

A characteristic feature of the Fibonacci chain is that a B atom is always flanked on both sides by A atoms as nearest neighbours, which is a type of local symmetry. This symmetry holds no matter where we take a B atom in the Fibonacci chain. This means that the value of q_B is precisely equal to unity, irrespective of the side of the B atom on which the A atom appears. Hence $p_B = 0$, and from relation (3) we get $q_A = 1/\tau$ and thus $p_A = (\tau - 1)/\tau$. The SRO parameters for the Fibonacci chain are thus uniquely determined.

For describing the effective medium in which the Fibonacci chain can be embedded, we now use the above values of the parameters in the CBLM theory given in [17], setting

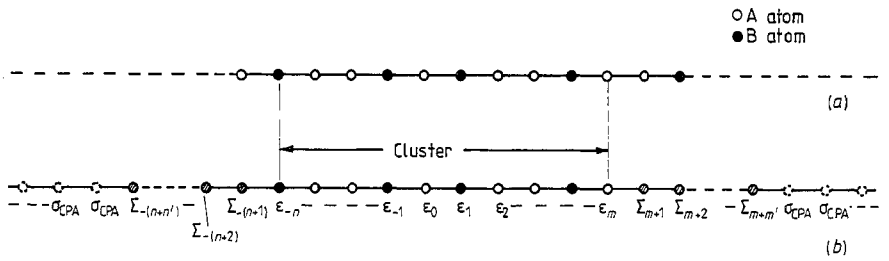

Figure 1. (*a*) The infinite Fibonacci chain. (*b*) Our model chain. The right- and the left-hand boundary atoms are respectively situated at the mth and nth sites from the origin. In this diagram $m = 5$ and $n = 4$.

the coordination number $Z = 2$. Beginning with a given atom, the concentrations of A and B atoms i generations away were shown to be given by

$$x_i = x + \Delta x f^i \qquad y_i = 1 - x_i \tag{4}$$

respectively. f is independent of i, and has the value $1 - q_A/y$. Putting in the values of q_A and y, we find the value of f in the present case to be $-1/\tau$. The value of Δx is y or $-x$ depending on whether the starting atom is of A or B type. Equation (4) giving the dependence of the concentration on the generation index essentially results from the self-avoiding nature of the paths in a Bethe lattice, and therefore holds in the case of a linear chain. Once we specify the cluster, the boundary atoms are also specified. Given a particular boundary atom, the probabilities of getting A and B atoms as its first, second, etc nearest neighbours outside the cluster are thus known from (4). Using these probabilities, the self-energy of the ith neighbour can be expressed as

$$\Sigma_{m+i} = \sigma_{CPA} + \langle T\rangle_i/(1 + \langle T\rangle_i G(\sigma_{CPA})) \tag{5}$$

where the boundary atom is situated at the mth site from the origin, which is a suitably chosen site within the Fibonacci cluster. Here, σ_{CPA} is the CPA self-energy and $\langle T\rangle_i = x_i T_A + y_i T_B$, $T_{A(B)}$ being the single-site scattering matrix elements, and $G(\sigma_{CPA})$ is the site-diagonal matrix element of the CPA Green function. In figure 1(*a*) we have indicated the infinite Fibonacci chain while our model Fibonacci chain is illustrated in figure 1(*b*). In terms of this effective medium, the site-diagonal matrix element of the Green function is given by

$$\langle 0|G(E)|0\rangle = [E - \varepsilon_0 - t(T_L + T_R)]^{-1} \tag{6}$$

where the state $|0\rangle$ corresponds to the chosen site within a large but finite-sized Fibonacci chain, whose boundaries are connected to the effective medium as defined above. The quantities T_R and T_L are defined as

$$\begin{aligned} T_{R(L)} = t/\Big[E - \varepsilon_{1(-1)} - t^2/\Big(E - \varepsilon_{2(-2)} - t^2/\ldots \\ \ldots/[[E - \varepsilon_{m(-n)} - t^2/\{E - \Sigma_{m+1(-n-1)} \\ - t^2/[E - \Sigma_{m+2(-n-2)} - t^2/\ldots/(E - \Sigma_{m+m'(-n-n')} \\ - tT(\sigma_{CPA}))\ldots]]\ldots\Big)\Big]. \end{aligned} \tag{7}$$

Here, the ε_i are the site energies of the atoms in the cluster whose domain is $-n \leqslant i \leqslant m$. Beyond the $(m + m')$th site on the right and $-(n + n')$th site on the left,

the site energies coincide with the CPA self-energy to within a small prescribed limit [17]. This limit sets the level of accuracy of the effective medium. The transfer matrix $T(\sigma_{\mathrm{CPA}})$ is given by

$$T(\sigma) = [E - \sigma \pm \sqrt{(E-\sigma)^2 - 4t^2}]/2t. \tag{8}$$

The LDOS is obtained from the expression

$$\rho(E) = -(1/\pi)\,\mathrm{Im}\langle 0|G(E)|0\rangle. \tag{9}$$

The average LDOS can be calculated in a straightforward way by computing the LDOS at the various sites within the cluster and then averaging them directly. An alternative method is to take the concentration-weighted average of the LDOS at A and B sites. The accuracy of the first method depends on the number of sites over which the averaging has been done, but the computation time follows a power law with the increase in the number of sites. The second method, however, is too crude, although the computation time is small. We have followed a compromise approach which does not require much computer time and yet retains a high level of accuracy. Considering up to the first neighbours of a particular site we see that with an A-type central atom we can have only clusters of the form AAB, BAA and BAB, while a B-type central atom can occur only within the cluster ABA, where all these atoms are members of a Fibonacci chain. For a given A-type central atom, the weights of the AAB, BAA and BAB configurations are respectively $p_{\mathrm{A}}q_{\mathrm{A}}$, $p_{\mathrm{A}}q_{\mathrm{A}}$ and q_{A}^2. These weights are to be normalised, since the forbidden configuration AAA has a non-zero weight p_{A}^2. However, for a B-type central atom, only the configuration ABA is allowed, the others being forbidden, and the weight of this configuration is unity since $q_{\mathrm{B}}^2 = 1$. Now we compute the LDOS of three A-type sites appearing in the three configurations mentioned above and average them with their respective weights to get the average LDOS at an A site. It is obvious that as long as we are only considering up to first-nearest neighbours, the average LDOS at a B site is directly given by the B-site LDOS. Finally, the average LDOS can be obtained from the concentration-weighted average of the average LDOS at A and B sites. We find that this averaging technique gives results that are very satisfactory.

Figure 2(*a*) is the plot of the LDOS at an A site for a typical configuration AAB, and in figure 2(*b*) we have plotted the average LDOS. Here the parameters of the Hamiltonian are taken to be $\varepsilon_{\mathrm{A}} = -\varepsilon_{\mathrm{B}} = 1$ and $t = -1$. One can easily check that a Fibonacci chain of finite order always forms a part of the infinite Fibonacci chain. Hence we make the choice that the cluster is a Fibonacci chain of finite order. We have observed that the positions of the bands as well as their shapes converge very rapidly to stable values with the increase of the cluster size. For instance, the LDOS for a cluster containing 610 atoms is found to differ from the LDOS for a Fibonacci cluster containing 987 atoms by 1 part in 10^3 on average, which is well within the limits of acceptable accuracy for the LDOS. Here we reproduce the results for the 14th generation Fibonacci chain having 610 atoms in the cluster. The study of both LDOS and averaged LDOS reveals that there exists a four-sub-band global structure, wherein each sub-band splits into three sub-bands. In fact, this four-sub-band structure, together with the splitting characteristics of the LDOS, is a global feature of every local environment in which a chosen sub-cluster—AAB, say—happens to be placed, although the value of the LDOS does depend on the environment, as is to be expected [15]. The widths of these sub-sub-bands are very small and a more detailed energy scan shows each of them to follow a hierarchy of splitting from one to three sub-bands until the gaps between them vanish. The DOS curves have no discontinuities, although they exhibit a lot of structure. The physical parameters used in

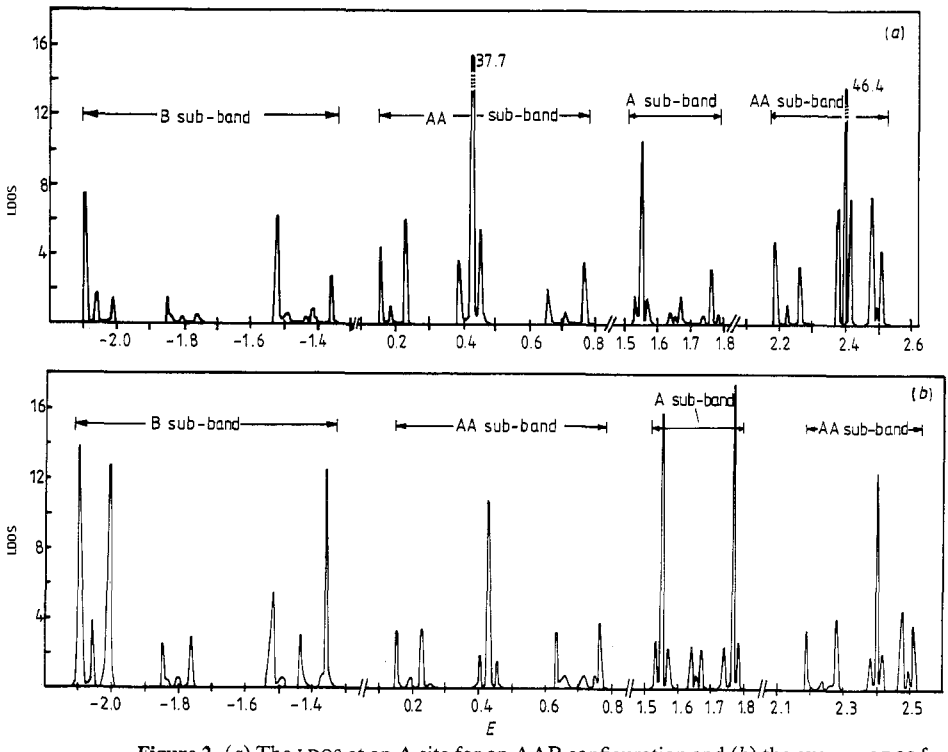

Figure 2. (*a*) The LDOS at an A site for an AAB configuration and (*b*) the average LDOS for a Fibonacci chain. The cluster is a 14th-generation Fibonacci chain containing 610 atoms. $\varepsilon_A = -\varepsilon_B = 1$ and $t = -1$.

the calculations presented here are taken to be the same as those used by Liu and Riklund [5], who studied the energy spectrum of a finite Fibonacci chain numerically for the on-site model. We have observed that the positions of the various bands as well as their widths agree quite closely with the results of Liu and Riklund. This agreement is found because the band positions and their widths are governed by the Hamiltonian parameters and also by the lattice structure. Niu and Nori [2] have suggested a two-sub-band global structure for the on-site model in an approximate scheme based on the RG method, but our method always yields a four-sub-band global structure even when the calculations are carried out with their values of the physical parameters. For disordered systems, it is well known that if there is a tendency to perfect long-range ordering, say, close to the binary limit [15], the levels try to push each other and gaps open up in the DOS. Hence we infer that the perfect long-range order in the Fibonacci chain is responsible for the large number of gaps in the DOS. The four-sub-band global structure is a characteristic of the on-site model. These sub-bands arise from the electronic levels of isolated A and B atoms and also from the bonding and anti-bonding levels of the AA cluster. The positions of these global sub-bands are indicated in figures 2(*a*) and (*b*). However, the hierarchical trifurcation of each sub-band is a characteristic of the Fibonacci lattice, and is observed in both on-site and transfer models. In figure 3 we have plotted the integrated averaged LDOS as a function of the Fermi energy. It shows that the fractional number of states under the B sub-band is almost equal to the concentration of B atoms, while the remaining fraction of states are distributed among the A sub-band and the two AA sub-bands. We have observed that the areas under the two AA sub-bands are equal. Figure 3 gives the distributions of states among the four global sub-bands. This figure also shows

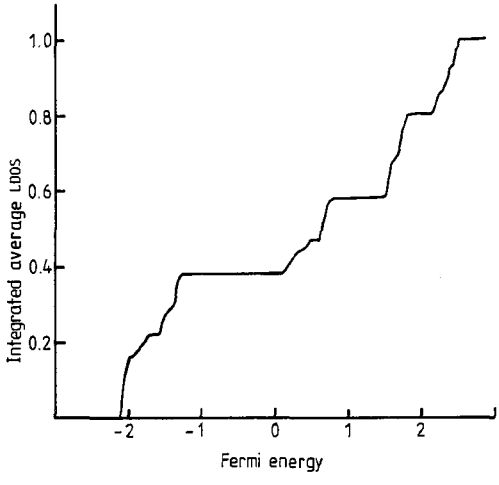

Figure 3. The integrated average LDOS as a function of the Fermi energy (the cluster size and the Hamiltonian parameters are the same as in figure 2).

that the total area under the DOS curve is unity, as expected.

Finally, we want to make the following comments regarding the present model. We have numerically observed that the Green function has the correct analytic behaviour for all values of energies. The LDOS can be calculated with an arbitrary degree of accuracy by just increasing the cluster size. So far, we have seen that the averaging procedure used here gives the average LDOS very well. However, it can be improved still further in a straightforward way by looking beyond the first neighbours. This we propose to investigate in the future.

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