Exact local Green function for phonons in a Fibonacci chain: a new real-space renormalisation group approach

LETTER TO THE EDITOR

Exact local Green function for phonons in a Fibonacci chain: a new real-space renormalisation group approach

Arunava Chakrabarti, S N Karmakar and R K Moitra

Saha Institute of Nuclear Physics, 92 Acharya Prafulla Chandra Road, Calcutta 700 009, India

Abstract. An exact real-space renormalisation group (RSRG) approach for the local Green function (LGF) for a quasi-periodic Fibonacci chain has been developed. The method has been used to study the local density of states (LDOS) for phonons, both in the on-site and transfer models. The scale factor in this work is τ^3, τ being the golden ratio. Apart from mapping a Fibonacci chain onto itself, our transformation accounts for the additional constraining symmetry, namely, that the local environment around the site at which the LGF is being found should remain invariant. The Cantor set-like behaviour of the energy spectrum results naturally from our alternative formulation.

Recent years have witnessed considerable activity, both theoretical and experimental, leading to the understanding of the structure and stability of quasi-crystals, first observed through the experiments of Schechtman and co-workers[1]. The idea of two-dimensional aperiodic tiling of a plane, first introduced by Penrose[2], provides an excellent conceptual tool for understanding the structure of actual three-dimensional quasi-crystals. Such systems are neither periodic in the sense of a perfect crystal, nor are they completely random, but in them the long-range bond-orientational order appears in perfect harmony with the observed icosahedral symmetry. This completely new topology results in exotic electronic structures, namely, the Cantor set energy spectrum, self-similar wavefunctions etc [3]. These properties are shared by quasi-crystals in any spatial dimension, and in particular by the one-dimensional version of quasi-periodic systems, which has received much attention during the last few years [4, 5]. Apart from the intrinsic interest in such one-dimensional systems because of their possible amenability to analytic study, there is the added interest that such systems have recently been prepared by appropriate stacking of thin semiconducting films [6]. Such samples are therefore likely to provide testing grounds in future for experimental verification of the various aspects of quasi-periodicity that are currently being studied theoretically.

   A well studied model of a one-dimensional system is the Fibonacci chain, on which considerable work has been done so far through the efforts of Ostlund and co-workers,

Kohmoto and co-workers and many others also (see [4, 5]). Both analytical and numerical methods have been employed to find out the multi-fractal nature of the wavefunctions and the scaling of the energy spectrum, though the number of exact results obtained are relatively few so far. Among the analytical techniques the most important one is the real-space renormalisation group (RSRG) scheme, first introduced by Kohmoto, Kadanof and Tang (KKT) [4]; it has been used by several authors [5] for studying the nature of the eigenfunctions in such systems. The KKT scheme mainly exploits an exact recursion relation between transfer matrices whose traces exhibit a non-linear dynamical mapping for a one-dimensional model described by a difference equation version of the Schrödinger equation. On the other hand, much less attention has been given so far to the study of local properties in one-dimensional quasi-periodic lattices [7–9]. In a Fibonacci chain every site is different from every other as far as the local topology is concerned and hence it is of extreme importance to study the environmental-dependent quantities such as the local density of states (LDOS), which are likely to reveal important information regarding the structure of quasi-crystals in general. For this, it is necessary to determine the local Green functions (LGF) at any arbitrary site on the Fibonacci chain. Since every atom in a Fibonacci chain sits in a different environment, the LGF is different at every site. This implies that each site in the chain has associated with it its own hierarchy of equations for the LGF. This situation is intrinsically different from the case of the eigenfunctions, where we have a *single* set of equations for the whole system [4]. Thus it is not possible to employ the RSRG scheme of KKT for studying the LGF.

Within the RSRG framework, a step in the right direction was recently taken by Ashraff and Stinchcombe [9], who discussed a decimation scheme for finding the LGF on a Fibonacci chain. This scheme maps the chain onto itself, thereby maintainings its global quasi-periodic character. However, it misses the most desired aspect of the RSRG transformation in this case, namely, that the Fibonacci chain must also be *locally invariant* around the site at which the LGF is to be found, the site itself remaining undecimated during the transformation. In fact, it can easily be checked that the hierarchy of equations for the Green functions for any chosen site does not remain invariant under the decimation transformation proposed by Ashraff and Stinchcombe (AS). Furthermore, this scheme identifies only three types of site in the chain, α, β and γ, depending on the possible nearest neighbours of the site, whereas it is well known that *every* site in any quasi-periodic system sits in a different environment if one looks beyond the nearest neighbours. Thus the α sites, for instance, are not equivalent to one another, and thus they do not share the same LGF. This is also true for the β and γ sites.

In this Letter we report a novel RSRG scheme for obtaining *exactly* the LGF at any arbitrary site of an infinite Fibonacci chain. Our method is free from all the shortcomings of the AS work, and in particular it takes adequate account of the local invariance requirements mentioned above. Using our approach we have determined the LDOS for phonons in a Fibonacci chain. For this, we develop a variant of the real-space decimation scheme used first by Southern and co-workers [10] and da Silva and Koiller [11]. As in the work of AS, the formulation of the present approach requires the consideration of three different types of mass, as well as two different coupling constants. Our method therefore automatically includes both the on-site and the transfer models as special cases, apart from being applicable to the more general and realistic situation when a combined model has to be considered.

Let us consider a linear chain of atoms in which long (L) and short (S) bonds are arrayed in the Fibonacci sequence. We suppose that the mass of the atom at an L–L vertex is m_1, that at an L–S vertex is m_2 and that at an S–L vertex is m_3. Since S–S bonds
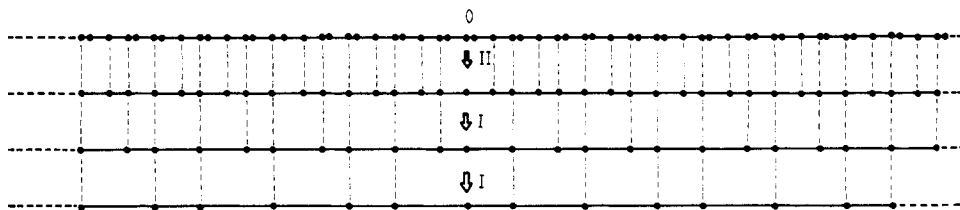
Figure 1. The central portion of a Fibonacci chain in the 12th generation containing 233 bonds with the key site marked '0'. We illustrate the appropriate sequence of transformations I and II necessary for the RSRG scheme. The key site in this case has a mass m_2.

do not appear in a Fibonacci chain, these three are the only possibilities. Let k_L and k_S respectively be the spring constants corresponding to a long and short bond. The equations for the Green functions have the form

$$\sum_j \left(\frac{W_{ij}}{m_i} - \omega^2 \delta_{ij} \right) G_{jk} = \delta_{jk} \tag{1}$$

where m_i is the mass of the ith atom and

$$W_{ij} = \partial^2 V / \partial u_i \, \partial u_j \tag{2}$$

and

$$V = \tfrac{1}{2} \sum_i k_{i,i+1} (u_i - u_{i+1})^2 \tag{3}$$

in the harmonic approximation. The LDOS at the jth site is given by

$$\rho_j(\omega) = (1/\pi) \, \text{Im} \, G_{jj}(\omega^2 + \text{i}0^+). \tag{4}$$

Considering figure 1, the set of equations (1) may be explicitly written out as

$$(k_L + k_S - m_2\omega^2)G_{00} = 1 + k_S G_{10} + k_L G_{-10}$$

$$(k_S + k_L - m_3\omega^2)G_{10} = k_S G_{00} + k_L G_{20} \tag{5}$$

$$(2k_L - m_1\omega^2)G_{20} = k_L G_{10} + k_L G_{30}$$
$$\vdots$$

and so on for both the right and left sides of the central site (i.e. the zeroth site) which is chosen to have mass m_2 in this case. The implementation of a decimation–renormalisation scheme demands that we remove a suitable set of sites from the above equations, such that the central site is left undecimated and the original environment of the central atom is kept invariant, with renormalised atomic masses and coupling strengths of course. This requirement is quite different from that in the case of the determination of the dispersion spectrum of a Fibonacci chain, where the chain has to be kept globally invariant under a RG transformation. In contrast, in the present case we have the additional constraint of keeping the local environment *also* invariant with respect to the chosen central site. Thus we need an altogether different RG scheme.

First of all, let us define the elementary RG transformations of the bonds L + S → L', L → S' and S + L → L', L → S', which we call transformations of type I and II

respectively. These are not equivalent transformations because of the intrinsic hand-edness of a Fibonacci chain. Transformation I is, in fact, identical to that used by AS. A very detailed and exchaustive examination of Fibonacci chains of various orders reveals the following striking factors. Firstly, in every generation it is possible to identify a special site, which we call a 'key site', whose environment remains invariant under a suitable three-step combination of transformations I and II listed above, while the site itself remains undecimated. This means that we are able to map a Fibonacci chain onto a segment of itself around the key site, which immediately leads to the desired RG scheme. In figure 1 we show a part of the original chain and the sub-chains that result after each step of decimation for the case under consideration. We have been able to detect three types of key site and have classified Fibonacci chains of different generations into three distinct classes, each class being characterised by a single key site which is a unique choice for that class. A notable feature of such classification is that the three classes described above exhibit the following closure property. The first application of an elementary transformation I or II maps one particular class onto the class of the previous generation. The second application of the decimation scheme maps this 'new' chain onto the chain belonging to the remaining class and the final step (I or II) brings back the configuration of the particular class with which we started originally. The decimation operations follow a well defined sequence for every class.

Now as far as the other sites are concerned, we find that they can always be mapped onto a segment around the key site using similar combinations of the elementary decim-ation steps I and II, the number of these steps being governed by the position of a site with respect to the key site in any particular generation. If, in a Fibonacci chain of any generation, we select a segment around the key site which represents a chain of the lowest order belonging to that particular class, then the configuration around any off-centre site in that segment can be transformed into the configuration around the key site of that class by a suitable three-step decimation. The chosen off-centre site now becomes the key site with renormalised mass and coupling constants. For a longer segment representing the next-highest-order generation around the same key site, the additional sites, which appear beyond the boundary of the lowest-order chain, can be transformed into the key site by a six-step decimation and so on. Once this is achieved, the RG procedure for those other sites may proceed in the same manner as in the case of the key site. We have checked these contentions using chains containing up to 46 368 bonds, and found them to be exactly true in every case. This gives us sufficient confidence that the RG scheme outlined above is universally true for Fibonacci chains of any length.

We give below the exact recursion relations obtained from the Green function equations (5) for the three masses and the spring constants obtained for a key site of mass m_2:

$$\varepsilon_1' = \varepsilon_2 - \frac{k_L^2 + k_S^2}{\varepsilon_3} - \frac{k_L^2 k_S^2}{\varepsilon_3^2(\varepsilon_1 - k_L^2/\varepsilon_3)} - \frac{k_L^4 k_S^2/[\varepsilon_3(\varepsilon_1 - k_L^2/\varepsilon_3)]^2 + k_L^2 k_S^2/\varepsilon_3^2}{\varepsilon_2 - k_S^2/\varepsilon_3 - k_L^2/(\varepsilon_1 - k_L^2/\varepsilon_3)}$$

$$\varepsilon_2' = \varepsilon_2 - \frac{k_L^2 + k_S^2}{\varepsilon_3} + \frac{k_L^2 k_S^2/\varepsilon_3^2}{\varepsilon_1 - k_L^2/\varepsilon_3} - \frac{k_L^2 k_S^2/\varepsilon_3^2}{\varepsilon_2 - k_S^2/\varepsilon_3 - k_L^2/(\varepsilon_1 - k_L^2/\varepsilon_3)}$$

$$\varepsilon_3' = \varepsilon_2 - \frac{k_S^2}{\varepsilon_3} - \frac{k_L^2 k_S^2/\varepsilon_3^2 + k_L^2}{\varepsilon_1 - k_L^2/\varepsilon_3} - \frac{k_L^4 k_S^2/[\varepsilon_3(\varepsilon_1 - k_L^2/\varepsilon_3)]^2}{\varepsilon_2 - k_S^2/\varepsilon_3 - k_L^2/(\varepsilon_1 - k_L^2/\varepsilon_3)}$$

$$k_L' = \frac{k_L^3 k_S^2/\varepsilon_3^2(\varepsilon_1 - k_L^2/\varepsilon_3)}{\varepsilon_2 - k_S^2/\varepsilon_3 - k_L^2/(\varepsilon_1 - k_L^2/\varepsilon_3)}$$
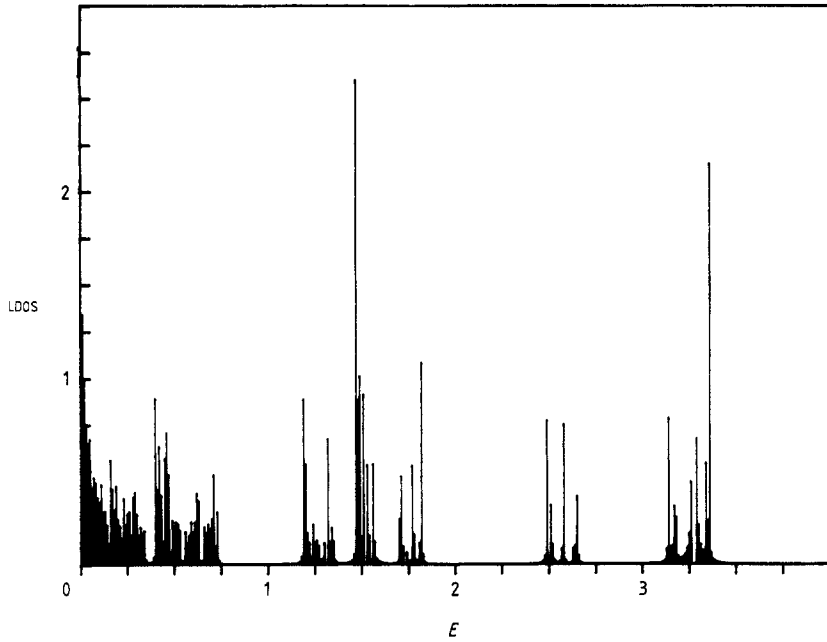
Figure 2. The LDOS at the key site with mass m_2 in the on-site model. $m_1 = m_3 = 1, m_2 = 2$ and $k_L/k_S = 1$.

$$k_S' = \frac{k_L^2 k_S}{\varepsilon_3(\varepsilon_1 - k_L^2/\varepsilon_3)}$$

where

$$\varepsilon_1 = m_1 \omega^2 - 2k_L$$

$$\varepsilon_2 = m_2 \omega^2 - (k_L + k_S)$$

$$\varepsilon_3 = m_3 \omega^2 - (k_S + k_L).$$

A closer look at the recursion relations shows that we have a stable fixed point at $k_L = k_S = 0$, so after infinite iterations we are left with a single pseudo-atom effectively decoupled from the rest. The local Green function at the specified site is then given by

$$G_{00} = 1/(-\varepsilon_2')$$

and hence the LDOS can easily be obtained. In figures 2 and 3 we give the LDOS for the on-site and transfer model respectively, and in figure 4 we present the results of the combined model. All the LDOS plots show the expected fragmented structures characteristic of such a chain. Since we know the entire spectrum, the positions of the band gaps can be exactly determined. Our results confirm the positions of the gaps obtained numerically by Odagaki and co-workers [3].

We have also examined the behaviour of the spring constants k_L and k_S under successive iterations of the recursion relations. In a periodic system the eigenfunctions are extended and the spring constants under renormalisation behave differently outside and inside the energy bands. For example, for energy values lying outside the band, that
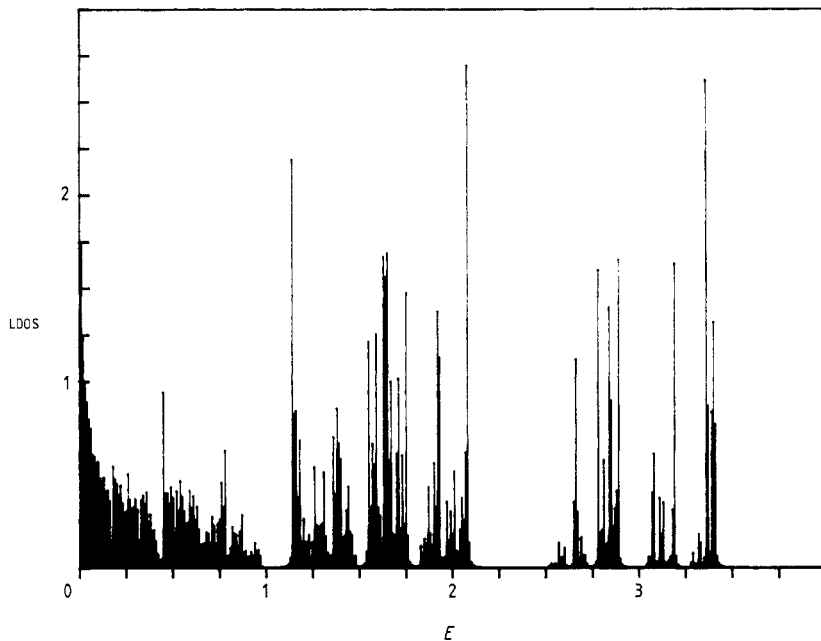
Figure 3. The LDOS at the key site with mass m_2 in the transfer model. $m_1 = m_2 = m_3 = 1$ and $k_L/k_S = 0.75$.
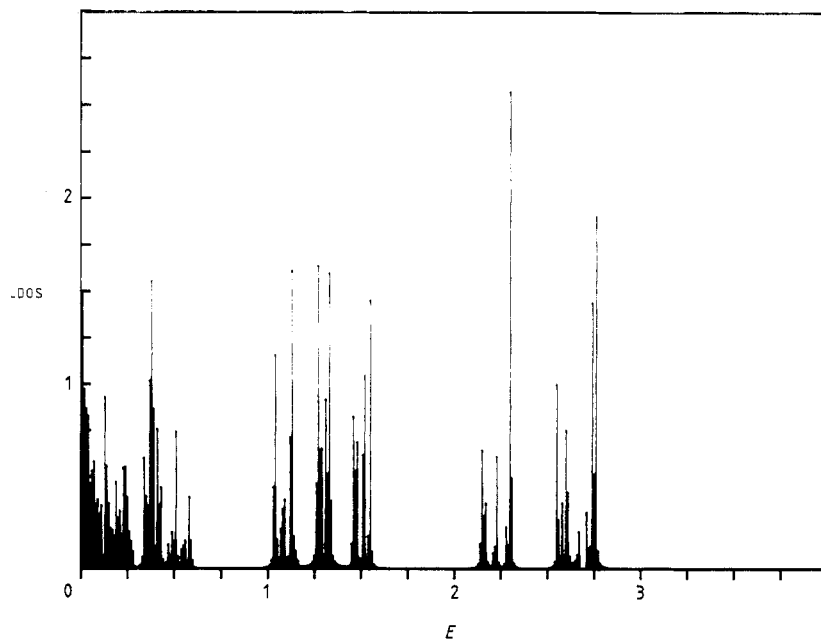
Figure 4. The LDOS at the key site with mass m_2 in the combined model. $m_1 = m_3 = 1, m_2 = 2$ and $k_L/k_S = 0.75$.

is within a gap, the k iterate to zero whether or not the energy contains an imaginary part [10]. But inside the band the k display oscillations for real values of the energy and flow to zero on adding even a very small imaginary part to the energy. In the case of a quasi-periodic chain we observe that the spring constants always go to zero under iteration for every energy whether or not the chosen energy contains an imaginary part. This again confirms the fact that all the energy levels of a quasi-periodic chain are isolated and the energy spectrum is a Cantor set.

In conclusion we would like to emphasise that we have described an *exact* decimation–renormalisation scheme for obtaining the local properties of a Fibonacci chain. We have demonstrated our approach by finding the LGF for phonons in an infinite Fibonacci chain. Interestingly, the present RG scheme involves the length scale τ^3, where τ is the golden ratio. In view of the three-cycle nature of the RG transformation, it is tempting to speculate that the trifurcating nature of the spectrum is intimately related to this basic RG step. It is now possible to obtain the off-diagonal Green functions by this method, and to study the conductivity for the pure Fibonacci chain as well as for the cases where impurities are present. The electronic case can be dealt with in an entirely analogous manner. A detailed RG analysis, together with the study of all these problems, will be presented in future publications.

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