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Exact real-space renormalization-group approach for the local electronic Green's functions on an infinite Fibonacci chain

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We present a new real-space renormalization-group (RSRG) scheme for finding exactly the local Green's functions (LGF) for electrons in a quasiperiodic Fibonacci chain. It has been possible to construct the RSRG transformation, which, apart from renormalizing the Fibonacci chain globally, also preserves the local environment around any chosen site at which the LGF is being found. The relevant scale factor in this work is τ^3, where τ is the golden ratio. The present work gives an alternative confirmation of the Cantor-set-like behavior of the energy spectrum of the Fibonacci chain.

Following the experimental discovery of icosahedral symmetry in the Al-Mn alloy by Shechtman *et al.*,[1] extensive research is being done to understand the structure and stability of quasicrystalline systems. Such systems can be thought of as being intermediate between a periodic structure and a disordered one, where icosahedral symmetry coexists with long-range bond-orientational order. The theoretical understanding of quasicrystalline structure is based on three-dimensional extensions of two-dimensional Penrose tiles[2] as discussed in the articles of Mackay[3] and Levine and Steinhardt.[4] The basic symmetries of these structures are quasiperiodicity, self-similarity, and local Penrose isomorphism; and these properties are common for quasicrystals in any spatial dimension. Therefore the study of quasicrystals even in one dimension should provide information about the spectral properties of such systems in general.

A Fibonacci chain is a one-dimensional version of Penrose tiles which has been the subject of extensive research during the past few years. In particular, interest in studying Fibonacci chains has increased considerably since Merlin *et al.*[5] succeeded in growing a quasiperiodic superlattice, which was then examined by x ray and Raman scattering technique. Both analytic and numerical methods have been employed so far for obtaining the Cantor-set energy spectrum, critical wave functions, and other exotic electronic properties, characteristic of such systems.[6,7] Among the analytic methods the real-space renormalization-group (RSRG) scheme developed by Kohmoto, Kadanoff, and Tang (KKT) (Ref. 8) has been widely used by many authors.[9,10] The KKT scheme mainly establishes a recursion relation between the transfer matrices on a Fibonacci chain and obtains the exact wave function only at zero energy ($E=0$). Another decimation scheme was proposed by Niu and Nori[11] on the transfer model of a Fibonacci chain to explain the hierarchical splitting of the energy spectrum. The theoretical calculations done so far mainly concentrate on the global structure of the energy spectrum and the scaling properties of wave functions. Comparatively speaking, much less attention has been given so far to the local electronic properties[12-14] of such one-dimensional quasiperiodic systems, such as the local density of states (LDOS). Because of the lack of periodicity, each atom in a Fibonacci chain has a different environment if one goes beyond the nearest neighbors. This is reflected in the hierarchy of equations for the local Green's function (LGF) corresponding to any chosen site in the chain, the LDOS being easily obtainable once the LGF is determined. It is found that every site is characterized by a different set of equations for the LGF, and this makes the LDOS different for every site. This situation is to be contrasted with the corresponding case of determination of the eigenfunctions of the Schrödinger equation on a Fibonacci lattice, where we have just a single hierarchy of equations. We shall presently discuss the fundamental reason for this difference, which necessitates the use of an altogether different RG scheme than that used by Kohmoto *et al.*[8]

Recently Ashraff and Stinchcombe (AS) (Ref. 13) have proposed a decimation-renormalization group scheme which relies on the mapping of a Fibonacci chain onto itself through the elimination of a suitable selection of sites. One must realize, however, that the requirement for a RG transformation for finding the *local* Green's function is much more stringent. While it is necessary that the Fibonacci chain must go over to a renormalized Fibonacci chain upon decimation, maintaining the *global* nature of the transformation, it is also additionally necessary that the *local* environment around the chosen site in the chain must map into itself with the site remaining fixed and undecimated. The equations for the LGF will remain invariant only under such a combined transformation, which would then constitute a proper RG transformation. The AS work does not take account for this local symmetry, and it can easily be checked that their decimation scheme does not preserve the invariance of the hierarchy of equations for the LGF for any site. Furthermore, they identify only three distinct sites in the chain, whereas each site has a different environment, and therefore leads to a different LGF.

In this paper we present a new RSRG scheme which enables us to determine the LGF *exactly* at any chosen site on a Fibonacci lattice, while respecting both the global and the local symmetry requirements of the transformations mentioned above. For this, we develop a variant of the real-space decimation scheme first used by Southern *et al.*[15] and da Silva and Koiller.[16] We illustrate our approach by considering the tight-binding Hamiltonian

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

where the hopping matrix element has two values t_L and t_S depending on whether a long (L) or a short (S) bond is being considered, these being arranged in the Fibonacci sequence. The general formulation of the RG transformation requires that we begin with three values of the site energies ε, namely, ε_1, ε_2, and ε_3, corresponding, respectively, to a L-L, L-S, and S-L vertex in a chain. Our method therefore automatically includes both the on-site and transfer models as special cases, apart from it being applicable to the more general and realistic situation when a combined model has to be considered. To fix our ideas, consider a segment of the chain shown in Fig. 1. We define first the elementary transformations

$$L+S\rightarrow L' \text{ and } L\rightarrow S'$$

and

$$S+L\rightarrow L' \text{ and } L\rightarrow S' ,$$

calling them transformations of type I and II, respectively. It is important to realize that these transformations are not identical because of an implied handedness in the construction of a Fibonacci lattice. This can also be checked by explicit construction of these two transformations. Transformation I is identical to the AS transformation. The application of the transformation of either type I or type II individually renormalizes the original chain to another Fibonacci chain of a smaller number of degrees of freedom, but fails to reproduce the exact bond-orientational environment around any arbitrarily chosen site, keeping that particular site undecimated. The local topology around any site now being completely different from the starting configuration, one fails to obtain the recursion relations for the parameters of the Hamiltonian. We arrive at the solution of this problem in the following manner.

An extensive examination of Fibonacci chains of various finite orders has resulted in the discovery of the following remarkable facts. First of all, in any generation, it is possible to identify *one* special site which we call the key site. The key site has the property that it is always possible, through a judiciously chosen *three-step* combination of the elementary transformations I and II listed above, to maintain invariant the entire arrangement of the bonds and sites around it, while itself remaining undecimated. In Fig. 1 we show a part of the original chain and the subchains that result after each step of decimation for the case under consideration. This immediately leads to the desired RSRG transformation for the key site. At every stage of decimation the number of degrees of freedom is reduced by a factor τ in the asymptotic limit, where τ is the golden mean, so that the length scale factor in the present RSRG scheme turns out to be τ^3. On further investigation we have found that there are three types of key sites altogether and, accordingly, have divided the Fibonacci chains of different generations into three distinct classes. Each class is characterized by a single type of key site which is a *unique* selection for that class. No two successive generations belong to the same class. These three classes exhibit a closure property discussed below. In any generation, the first operation of the three-step decimation scheme maps the entire configuration around the key site of a particular class onto the configuration around the key site of the class characterizing its previous generation. The second decimation step maps the resulting chain onto the chain belonging to the remaining class and, the final step reproduces the environment of the original class with which we started. At each stage of decimation the key site and its neighbors belonging to one particular class are transformed into the key site and its neighbors of another class with renormalized values of site energies and hopping integrals.

Now, as far as the sites other than the key site in any generation are concerned, we find that the application of the elementary transformations I and II in a suitable sequence transform the entire configuration around an arbitrarily chosen site into the configuration around the key site of the particular generation. The originally chosen site now becomes the key site of that generation. The resulting new chain has renormalized site energies and hopping integrals. The problem thus boils down to that of solving exactly the key site problem already discussed with the above renormalized Hamiltonian parameters. The number of decimation steps required for getting the key-site configuration is not always three, but depends on the position of the chosen site with respect to the key site in that generation. Exhaustive search for appropriate decimation schemes for such sites provides a most interesting solution to this problem. If, in a long Fibonacci chain belonging to a certain class we concentrate on a finite segment around the key site which represents the lowest-order Fibonacci chain of that class, then all the other sites in this segment can be transformed so as to have the key-

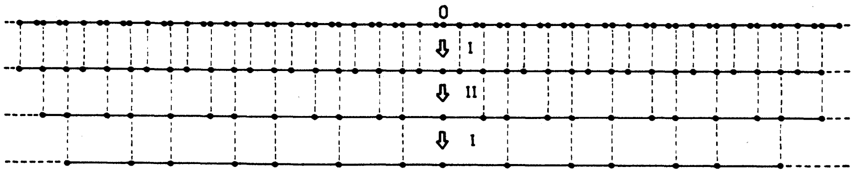

FIG. 1. The central portion of a Fibonacci chain in tenth generation containing 89 bonds with the key site marked "0". We illustrate here the appropriate sequence of transformations I and II necessary for the RSRG scheme. The site energy at the key site in this case is ε_3.

site configuration of that class through a three-step combination of schemes I and II. If we now concentrate on a larger segment around the key site which represents the next-higher-order chain in that particular class, then the additional sites beyond the lowest-order segment can be transformed to achieved the key-site configuration of the same class through a six-step decimation and so on. Once this is done, the RSRG operation may proceed in the same manner as in the case of the key site. We have checked these contentions to be exactly valid for chains containing up to 46 368 bonds. We may therefore conclude with complete confidence that the RSRG scheme outlined above is universally true for Fibonacci chains of any length.

We now proceed to obtain the recursion relations for the Hamiltonian parameters. We start by explicitly writing down the Green's function equations around a chosen key site of site energy ε_3 corresponding to the chain depicted in Fig. 1 and obtain the following hierarchy of equations for the Green's functions:

$$\begin{aligned}
&\cdots\\
&(E-\varepsilon_3)G_{-30}=t_L G_{-20}+t_S G_{-40}\,,\\
&(E-\varepsilon_1)G_{-20}=t_L G_{-10}+t_L G_{-30}\,,\\
&(E-\varepsilon_2)G_{-10}=t_S G_{00}+t_L G_{-20}\,,\\
&(E-\varepsilon_3)G_{00}=1+t_L G_{10}+t_S G_{-10}\,, \qquad (2)\\
&(E-\varepsilon_1)G_{10}=t_L G_{00}+t_L G_{20}\,,\\
&(E-\varepsilon_2)G_{20}=t_L G_{10}+t_S G_{30}\,,\\
&(E-\varepsilon_3)G_{30}=t_S G_{20}+t_L G_{40}\,,\\
&\cdots
\end{aligned}$$

and so on.

We obtain the following recursion relations:

$$\varepsilon_1'=\varepsilon_3+Z+\frac{t_L^2}{E-Y}+\frac{t_L^2 Z}{X(E-\varepsilon_2)}\left[\frac{t_L^2}{(E-Y)^2}+1\right], \qquad (3)$$

$$\varepsilon_2'=\varepsilon_3+Z+\frac{t_L^2}{E-Y}+\frac{t_L^2 Z}{X(E-\varepsilon_2)}\,, \qquad (4)$$

$$\varepsilon_3'=\varepsilon_3+Z+\frac{1}{E-Y}\left[\frac{t_L^2 Z}{E-\varepsilon_2}+t_L^2\right] + \frac{t_L^4 Z}{X(E-\varepsilon_2)(E-Y)^2}\,, \qquad (5)$$

$$t_L'=\frac{t_L^3 Z}{X(E-\varepsilon_2)(E-Y)}\,, \qquad (6)$$

$$t_S'=\frac{t_L^2 t_S}{(E-\varepsilon_2)(E-Y)}\,, \qquad (7)$$

where

$$X=E-\left[\varepsilon_3+\frac{t_L^2+t_S^2}{E-\varepsilon_2}+\frac{t_L^2 t_S^2}{(E-\varepsilon_2)^2(E-Y)}\right],$$

$$Y=\varepsilon_1+\frac{t_L^2}{E-\varepsilon_2}\,,$$

$$Z=\frac{t_S^2}{E-\varepsilon_2}\,.$$

The recursion relations reveal that the hopping terms t_L and t_S flow to zero on successive iterations so that after infinite iterations we are left with a single "pseudoatom" having a site energy ε_3^*. We then obtain the LGF at the chosen key site as

$$G_{00}=1/(E-\varepsilon_3^*) \qquad (8)$$

and the LDOS can be easily obtained. We illustrate in Figs. 2–3 the LDOS at the above site. In Figs. 2 and 3 we present the results for on-site and transfer models, respectively, while the LDOS for the combined model is given in Fig. 4. We have checked the results for the on-site and transfer models using an alternative method based on the cluster Bethe lattice framework[14] and also with the numerical works.[7] The four-subband structure in Fig. 2 shows the characteristics of the on-site model.[11] These subbands arise from the electronic levels of isolated A ($\varepsilon_A=1$) and $B(\varepsilon_B=-1)$ atoms and from the bonding and antibonding levels of the AA cluster. Niu and Nori[11] pointed out that in the transfer model the three global subbands correspond to the energy values $E=0$ and $E=\pm t_S$. The hierarchical splitting of each subband both in the on-site and the transfer models is a characteristic of the Fibonacci chain.

The sequence of transformations for the two other key sites with site energies ε_1 and ε_2 are I-I-II and II-I-I, re-

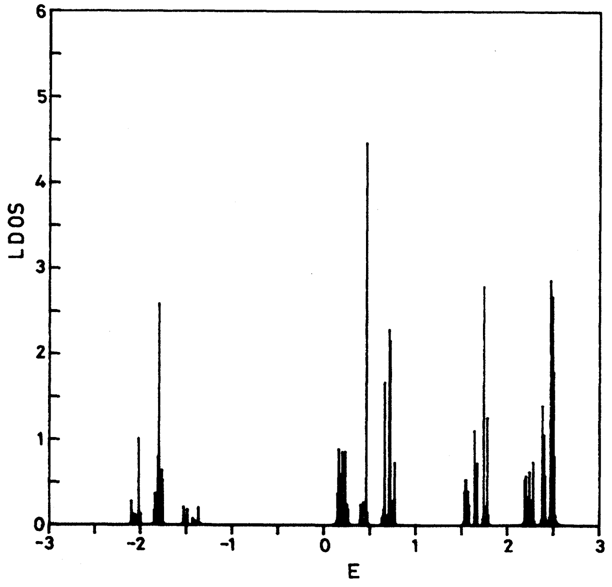

FIG. 2. The LDOS (arbitrary units) at the key site with site energy ε_3 in the on site model. $\varepsilon_1=-\varepsilon_2=\varepsilon_3=1$ (in units of t_L), $t_S/t_L=1$.

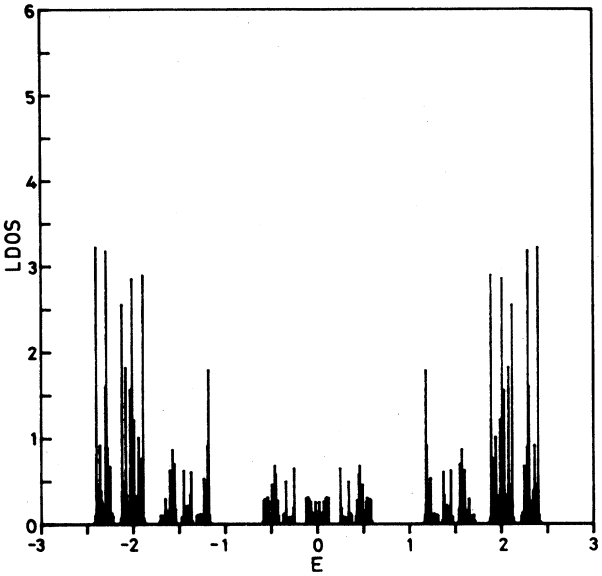

FIG. 3. The LDOS (arbitrary units) at the key site with site energy ε_3 in the transfer model. $\varepsilon_1=\varepsilon_2=\varepsilon_3=0$ (in units of t_L), $t_S/t_L=1.5$.

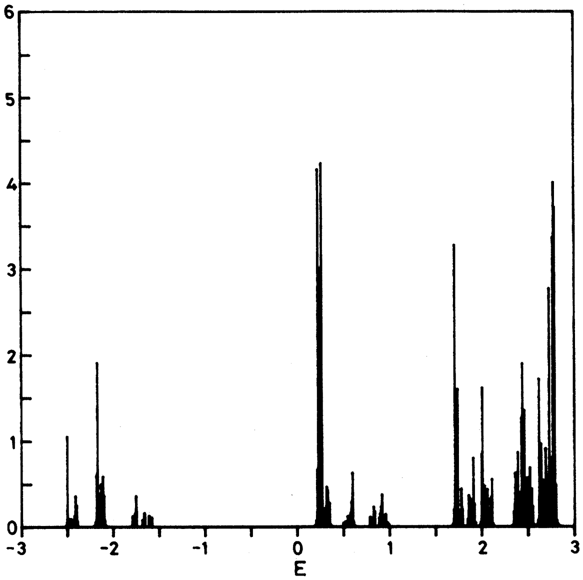

FIG. 4. The LDOS (arbitrary units) at the key site with site energy ε_3 in the combined model. $\varepsilon_1=-\varepsilon_2=\varepsilon_3=1$ (in units of t_L), and $t_S/t_L=1.5$.

spectively. It is then straightforward to obtain the LGF for them by applying the appropriate sequence. The LDOS will be different in each case.

We have studied the behavior of t_L and t_S under the RG transformation in some detail. As expected, the behavior is quite different from that in a periodic system. In a periodic system if a small imaginary part is added to the energy, the hopping integral under renormalization goes to zero inside the band. For real values of the energy the hopping term oscillates within the band without showing any sign of convergence.[15] Outside the band the t's however flow to zero whether the energy contains an imaginary part or not. But for a Fibonacci lattice we have observed that t_L and t_S flow to zero under RSRG operation for all values of energy, real or complex. This clearly shows that for such systems all the energy levels are discrete, that is, the spectrum is a Cantor set having zero Lebesgue measure.

In conclusion, we would like to emphasize that we have been able to discover a new decimation scheme for an infinite Fibonacci chain which correctly brings out the local features exactly. The present formulation is sufficiently general that the results for the on-site and transfer models come out as special cases. This scheme enables us to study various local properties which depend on the local topology of such quasiperiodic systems. A novel feature of this scheme is that it involves an irrational scale factor τ^3. We have found that the off-diagonal Green's functions can also be exactly calculated by this method, and hence, it is possible to study the conductivity for the Fibonacci chain, both for the pure system and also in presence of impurity. A study of all these problems, together with a detailed RG analysis of the scaling of the Green's functions will be published elsewhere.

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