Topological reduction of tight-binding models on branched networks

P. Buonsante,* R. Burioni,† and D. Cassi‡
Dipartimento di Fisica, Università degli Studi di Parma and Istituto Nazionale per la Fisica della Materia, Unità di Ricerca di Parma, Parco Area delle Scienze 7/a, 43100 Parma, Italy

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Noninteracting excitations on a generic discrete structure are described by means of a single-band tight-binding Hamiltonian. Despite the simplicity of the model, topological inhomogeneity gives rise to nontrivial spectral features. At the same time the lack of regularities makes the spectral analysis a rather hard task, since powerful tools such as Fourier transform are ruled out. In this paper we introduce a rigorous analytical technique, based on topological methods, for the exact solution of this problem in the case of branched structures. We provide some examples illustrating the technique.

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I. INTRODUCTION: THE ROLE OF TOPOLOGY

The tight-binding Hamiltonian was originally introduced to deal with electronic excitations in solid materials but it was soon extended to the study of many other kinds of excitations.[1] The environment where these excitations take place essentially consists of a collection of elementary building blocks arranged into a network. These building blocks are typically atoms, but they can also consist of more complex structures.[2,3]

When the network is regular and periodic, as in crystals, it is possible to isolate an elementary cell from which all the features of the system stem. At length scales much higher than the cell's size these features depend uniquely on the dimensionality of the cell's packing. Periodicity, as well as any other strong regularity arising from simple group properties,[4] is particularly useful in the analysis of the spectral features of the system. It makes it possible to introduce a (pseudo) wave vector **k** that labels many quantities of interest, such as the energy or the Green's functions.[5] When no periodicity is present, a lattice cannot be used to describe a discrete structure and there is no such simple labeling for the physically interesting quantities.

In this paper the spectral properties of a single-band tight-binding model applied to inhomogeneous structures are investigated. In order to analyze the features strictly arising from the topology of their arrangement we will simplify as much as possible the "internal structure" of the building blocks. The resulting model is simple yet rich, in that it retains the basic elements for a qualitative study of the effects of topology on the spectral features.[6,7] In this framework we will illustrate an analytical technique, which we call *bud reduction*, applicable to the large class of branched networks. As its name suggests it makes it possible to account for the spectral features stemming from an entire substructure off-branching from a site of a given network, by reducing it to what we call its *bud*. This operation is a sort of topological renormalization, in the sense that the presence of an entire substructure is accounted for by means of an on-site potential of geometrical origin. Since it is applicable also to structures that have already undergone a partial bud reduction, this technique proves to be very efficient on recursively defined structures. Indeed recursivity is of great help, since it allows for relations in closed form, but it is not a requirement of the technique. A deeper understanding of the features arising from topological arrangement is gained, in that the spectral properties of a complex structure are explicitly expressed in terms of the same properties of its simpler parts. The knowledge thus gained can possibly be exploited in designing networks displaying the desired spectral features.

The present paper is organized as follows. Section II briefly deals with the mathematical representation of discrete networks, from the topological point of view. A number of useful definitions are also given there. In Sec. III we introduce our tight-binding model, generalized to the case of an arbitrary network. In Sec. IV we review some mathematical tools that allow the computation of the spectrum of such an arbitrary network, independent of its symmetries and regularities. In Sec. V we describe bud reduction and provide numerous examples that clarify the technique and its application. Section VI consists of our conclusions.

II. REPRESENTATION OF AN ARBITRARY DISCRETE NETWORK: GRAPHS

When no periodicity is present a lattice cannot be used to describe a discrete structure, the appropriate choice being a graph.[8] A graph, $\mathcal{G}=\{\Sigma,\Lambda\}$, consists of a set of points, or sites Σ and a set of links Λ connecting the sites pairwise. In the present paper lowercase italic letters $i,j,k,\ldots$, will denote the sites of a network, and pairs of lowercase letters enclosed in parentheses (h,k) will denote the link joining the relevant sites. From an algebraic point of view a graph is completely described by what is called its *adjacency matrix*. Every entry of this matrix corresponds to a couple of sites of the network, and it equals one if and only if this couple is joined by a link, otherwise it is zero,

$$A_{ij}=\begin{cases}1 & \text{if } (i,j) \text{ is a link of the graph}\\ 0 & \text{otherwise.}\end{cases} \tag{1}$$

The sum of the elements in the kth row or column of the adjacency matrix gives the so called *coordination number* of site k, namely, the number of its nearest neighbors $z_k \equiv \Sigma_h A_{hk}=\Sigma_h A_{kh}$.

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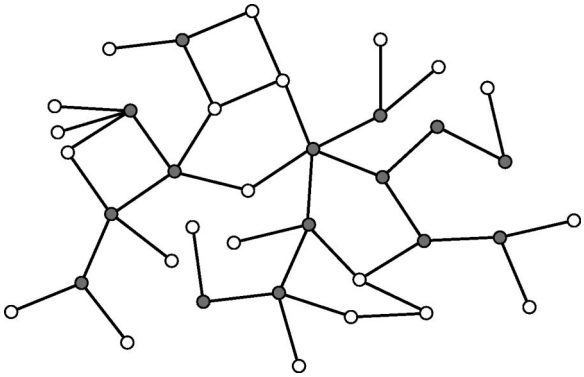

FIG. 1. Graph of a generic network. Filled circles denote branching sites, i.e., sites that are the unique intersection of any two connected subgraphs. Unfilled circles denote nonbranching sites.

Any sequence of consecutive links, $(i,h),(h,k),\ldots,(l,m),(m,j)$, is referred to as a *path* on the graph. In the following a path starting at site i and ending at site j will be denoted by the symbol $\mathcal{P}_{ij}$. In general such a path may reach its ending site j also at an intermediate step. When the path never passes through its ending site at an intermediate step it will be denoted by the symbol $\mathcal{F}_{ij}$.

The bud-reduction technique, which we will illustrate in Sec. V, can be performed at sites of the graph called *branching sites*. A site * of a graph $\mathcal{G}$ is a branching site if it is the only intersection of any two connected subgraphs $\mathcal{B}_1=\{\Sigma_1,\Lambda_1\},\mathcal{B}_2=\{\Sigma_2,\Lambda_2\}$ of $\mathcal{G}=\{\Sigma,\Lambda\}$; in mathematical terms,

$$\Sigma_1\cup\Sigma_2=\Sigma,\quad \Lambda_1\cup\Lambda_2=\Lambda,$$
$$\Sigma_1\cap\Sigma_2=\{*\},\quad \Lambda_1\cap\Lambda_2=\varnothing. \tag{2}$$

Any two subgraphs joined by a branching site are referred to as *branches*. What makes a branching site peculiar is the fact that any path joining sites on different branches is forced to pass through it. Figure 1 illustrates the concept of branching site.

III. TIGHT-BINDING MODEL FOR GENERIC STRUCTURES

In the following we will deal with a tight-binding Hamiltonian of the form

$$H_{ij}^{\mathrm{TB}}=tA_{ij}+az_i\delta_{ij}, \tag{3}$$

describing noninteracting excitations (typically electrons) on a generic structure represented by the adjacency matrix A. The off-diagonal term, containing the so-called *hopping parameter t*, and the adjacency matrix is referred to as *hopping term*. The diagonal term, containing the so-called *local parameter a*, and the coordination matrix $Z_{ij}=z_i\delta_{ij}$, is referred to as *local term*. The overall product az_i is usually referred to as the *one-site energy* at site i. A Hamiltonian such as Eq. (3) can be obtained starting from the first quantization Hamiltonian for a quantum particle experiencing an "atomic" potential $V_i(\mathbf{r})=V(\mathbf{r}-\mathbf{r}_i)$ at each site i of a discrete structure $H=\mathbf{p}^2/2m+\Sigma_i V_i(\mathbf{r})$. This can be done[9] through some approximations: the wave functions are assumed to be linear combinations of atomic orbitals; each atomic site is assumed to contribute with a single spherically symmetric orbital; these atomic orbitals are assumed to have nonzero overlap only if they come from adjacent atomic sites. In spite of the approximations that it has undergone, the model described above is nevertheless rich and capable of displaying the features arising from the topological arrangement of the structure. We remark the fact that the topology of the structure affects the Hamiltonian (3) both in the hopping term, through the adjacency matrix, and in the local term, in the form of a local potential depending on the site coordination. On a homogeneous network, such as a periodic lattice with homogeneous elementary cell, the local term is site independent and it can be dropped without loss of generality, since it simply results in a rigid shift of the spectrum. For a generic structure this cannot be done, and moreover there is no natural tool such as the Fourier transform for the diagonalization of the Hamiltonian. Hamiltonians of the form (3) are widely used. They describe noninteracting excitations in ordered or disordered solids.[1] The so-called *Hückel Hamiltonian* is a special case of Eq. (3) for vanishing local parameter. Due to its simplicity and to its content in topological information it is widely used in chemistry as a qualitative guide for planning and interpreting experiments.[8] The Schrödinger operator for discrete-space quantum mechanics[10] is also a special case of Eq. (3). We recall that the building blocks placed at the sites of the discrete network described by A can be structures more complex than single atoms, such as groups of atoms within molecules,[2] or even quantum devices, such as Josephson junctions in the weak coupling limit.[11] In the following we are not going to consider disorder, but only the effects of topological inhomogeneity[6] on the spectral features of the Hamiltonian (3).

IV. GREEN'S FUNCTIONS AND LOCAL DENSITY OF STATES

An approach to the spectrum of the Hamiltonian (3) alternative to direct diagonalization is based on the so-called *local density of states* (LDOS), which is related to Green's functions by the formula[12]

$$\rho_i(\omega)=-\frac{1}{\pi}\lim_{\epsilon\to 0}\mathrm{Im}[G_{ii}(\omega+i\epsilon)], \tag{4}$$

where the subscripts refer to a generic site i of the structure. We point out that most of the quantities we will introduce carry an explicit site dependence, which in the case of perfect crystals with simple primitive cell usually drops, due to the spatial homogeneity. The Green's function (GF) is defined by

$$G(\omega)=[\omega-H]^{-1}=[\omega-Za-tA]^{-1}, \tag{5}$$

where $Z_{ij}=z_i\delta_{ij}$. Denoting $|i\rangle$ the eigenfunction of the position operator at site i and $|\phi_k\rangle$ the eigenfunction of the Hamiltonian operator relevant to the eigenvalue ω_k, $H|\phi_k\rangle=\omega_k|\phi_k\rangle$, one can write $G_{ij}(\omega)\equiv\langle i|G(\omega)|j\rangle$

$=\Sigma_k\langle i|\phi_k\rangle\langle\phi_k|j\rangle(\omega-\omega_k)^{-1}$. Plugging this result into Eq. (4) and recalling that $\lim_{\epsilon\to 0}\mathrm{Im}(\omega\pm i\epsilon)^{-1}=\mp\pi\delta(\omega)$ one gets

$$\rho_i(\omega)=\sum_k \delta(\omega-\omega_k)|\langle i|\phi_k\rangle|^2. \tag{6}$$

The normalization of the eigenfunctions of the position operator and the completeness of the Hamiltonian's eigenfunctions yield the normalization of the LDOS. Equation (6) sheds light on the significance of the LDOS at site *i*. It is a sort of projection on that site of the density of states (DOS), $\rho(\omega)=\Sigma_k\delta(\omega-\omega_k)$. The DOS is recovered by simply summing the LDOS over all sites.

Simple algebraic manipulations of Eq. (5) yield

$$G_{ij}(\omega)=\frac{1}{\omega-z_j a}\sum_{k=0}^{\infty}[(\omega-Za)^{-1}At]_{ij}^k$$
$$=g_j\sum_{k=0}^{\infty}t^k\sum_{h_1,\ldots,h_{k-1}}g_iA_{ih_1}g_{h_1}A_{h_1h_2}\cdots g_{h_{k-1}}A_{h_{k-1}j}, \tag{7}$$

where $g_i(\omega)\equiv(\omega-z_i a)^{-1}$ is often referred to as *locator*[1,13–15] at site *i*, and it is nothing but the limit of the GF G_{ii} for vanishing hopping parameter,

$$\lim_{t\to 0}G_{ij}(\omega)=\frac{1}{\omega-z_i a}\delta_{ij}=g_i(\omega)\delta_{ij}. \tag{8}$$

This can easily be shown by means of Eq. (5), simply by observing that $\omega-H=\omega-aZ$ is a diagonal matrix when the hopping term vanishes, i.e., when the "atoms" of the structure are isolated from each other. For this reason we refer to $g_i(\omega)$ as the *atomic* GF at site *i*. Since the chain of adjacency matrix's elements $A_{ih_1}A_{h_1h_2}\cdots A_{h_{k-1}j}$ in Eq. (7) is nonvanishing only if $\{i,h_1,h_2,\ldots,h_{k-1},j\}$ is a connected *k*-step path joining the sites *i* and *j*, the GF $G_{ij}(\omega)$ can be viewed as a weighed sum over the paths $\mathcal{P}_{ij}$ joining *i* and *j*,

$$G_{ij}(\omega)=g_j\sum_{\mathcal{P}_{ij}}\prod_{(h,k)\in\mathcal{P}_{ij}}p_{hk}, \tag{9}$$

where $p_{hk}(\omega,t,a)=tg_h(\omega,a)$ is the contribution relevant to the step (h,k). Due to the extreme simplicity of the present model this quantity is a function only of the site from which the step is taken. In a more refined model the hopping parameter would be a link variable t_{hk} and this explains the dependence of p_{hk} on both of the sites involved in the step. Note that p_{hk} is a dimensionless quantity. Thus the LDOS is a local quantity, in the sense that it refers to a single site of the structure, but it takes into account the whole structure. This is because it depends on a GF, which is a weighed sum over all possible closed paths passing through the site under examination. The function

$$\Gamma_{ij}(\omega)=\sum_{\mathcal{P}_{ij}}\prod_{(h,k)\in\mathcal{P}_{ij}}p_{hk} \tag{10}$$

appearing in Eq. (9) is related to the generating function[16] $\tilde{P}_{ij}(\lambda)$ for a random walk (RW) with probability $\overline{p_{hk}}$ of taking the step (h,k). The function

$$\gamma_{ij}(\omega)=\sum_{\mathcal{F}_{ij}}\prod_{(h,k)\in\mathcal{F}_{ij}}p_{hk}, \tag{11}$$

built using only paths constrained as described in Sec. II, is in turn related to the generating function for the probability of first arrival $\tilde{F}_{ij}(\lambda)$.

$$\Gamma_{ij}(\omega)=\delta_{ij}+\gamma_{ij}(\omega)\Gamma_{jj}(\omega). \tag{12}$$

When the last site is the same as the first this reads

$$\Gamma_i(\omega)=\frac{1}{1-\gamma_i(\omega)}, \tag{13}$$

where $\Gamma_i(\omega)\equiv\Gamma_{ii}(\omega)$ and $\gamma_i(\omega)\equiv\gamma_{ii}(\omega)$.

We mention that the expansion (7) for the GF and the function $\gamma_i(\omega)$ of Eq. (11) are well-known mathematical tools. They are referred to as *locator expansion*[17] or *renormalized perturbation expansion*[18] and *renormalized interactor*[17] or *self-energy*,[18] respectively.

V. BUD REDUCTION

The analogous of formula (13) in the framework of RW is well known and is due to the factorization properties of the generating functions $\tilde{P}_{ii}$ and $\tilde{F}_{ii}$. Since the proof line for the bud-reduction technique is very similar, in the following Eq. (13) is proved employing a path technique. First of all we label all the relevant paths in some definite though arbitrary sequence for enumerating purposes. Thus let $\mathbf{P}_i=\{\mathcal{P}_{ii}^{(n)}\}_{n=1}^N$ be the set of all unrestricted paths starting and ending at site *i*, and let $\mathbf{F}_i=\{\mathcal{F}_{ii}^{(n)}\}_{n=1}^{\tilde{N}}$ be the subset of $\mathbf{P}$ consisting of the paths restricted as explained in Sec. II. Note that both *N* and $\tilde{N}$ may be possibly infinite. Let $\bowtie$ denote the operation of joining two paths. The only requirement for this operation is that the starting site of the second path is the same as the ending point of the first one. For instance $\mathcal{P}_{ij}\bowtie\mathcal{P}_{jk}$ is a path starting at *i* and ending at *k*. Let

$$p(\mathcal{P})=\prod_{(h,k)\in\mathcal{P}}tg_h \tag{14}$$

be a function of paths. The following equality holds:

$$p(\mathcal{P}_{ij}\bowtie\mathcal{P}_{jk})=p(\mathcal{P}_{ij})p(\mathcal{P}_{jk}). \tag{15}$$

As already pointed out $\mathbf{F}_i\subset\mathbf{P}_i$. Moreover any concatenation of elements in $\mathbf{F}_i$ is in $\mathbf{P}_i$. More precisely for any $\mathcal{P}_{ii}^{(h)}\in\mathbf{P}_i$ there exists a subset of $\mathbf{F}_i$, $\{\mathcal{F}_{ii}^{(k)}\}_{k=1}^n$, such that $\mathcal{P}_{ii}^{(h)}=\mathcal{F}_{ii}^{(1)}\bowtie\mathcal{F}_{ii}^{(2)}\bowtie\cdots\bowtie\mathcal{F}_{ii}^{(n)}$. Here *n* is nothing but the number of times the path $\mathcal{P}_{ii}^{(h)}$ reaches site *i*. Note that the elements of the subset of $\mathbf{F}_i$ are not necessarily all distinct. Thus, for any *h*, $p(\mathcal{P}_{ii}^{(h)})$ is the product of factors of the $p(\mathcal{F}_{ii}^{(k)})$ kind, each raised to some positive integer power $n(k)$. At this point it is easy to understand that the following formal equalities, which yield Eq. (13), hold:

$$\Gamma_i=\sum_{k=1}^{N} p(\mathcal{P}_{ii}^{(k)})=\sum_{h=0}^{\infty}\left[\sum_{l=1}^{\tilde{N}} p(\mathcal{F}_{ii}^{(l)})\right]^h=\sum_{h=0}^{\infty}\gamma_i^h=\frac{1}{1-\gamma_i}. \tag{16}$$

Now let us focus on the branching point. Let * be a branching point splitting the graph $\mathcal{G}$ into two branches as in Eq. (2). In the following we are going to show that the evaluation of the GF at any site of one of the branches can be equivalently performed by pruning out the other branch, provided that the atomic GF at the branching point is changed into an appropriate function. It will turn out that the appropriate new atomic GF is nothing but the GF of the pruned branch at the branching site. In formula,

$$G_{ii}=G_{ii}^{\mathcal{T}}|_{g_*=G_{**}^{\mathcal{B}}}, \tag{17}$$

where $\mathcal{T}$ and $\mathcal{B}$ denote, respectively, the branch containing i, which we call the *trunk* of the structure, and the branch off-springing from the branching site *. As superscripts, these letters denote restriction to the relevant substructure. First of all we consider the GF at the branching site *. Since the paths involved in γ_{**} never go through * at an intermediate step, they take place entirely either on $\mathcal{T}$ or on $\mathcal{B}$. Thus γ_{**} is the sum of two terms,

$$\gamma_*=\sum_{\mathcal{P}_{**}\in\mathcal{T}} p(\mathcal{P}_{**})+\sum_{\mathcal{P}_{**}\in\mathcal{B}} p(\mathcal{P}_{**})=\gamma_*^{\mathcal{T}}+\gamma_*^{\mathcal{B}}. \tag{18}$$

From each $p(\mathcal{P}_{**})$ appearing in Eq. (18) it is possible to factor out a term g_*. Thus g_* appears in γ_{**}, γ_{**}^{T}, and γ_{**}^{B} only as an overall factor. This means that g_* can be changed into another function, say $\bar{g}_*$, through the simple multiplication by the factor $g_*^{-1}\bar{g}_*$. For instance,

$$\gamma_*(\omega)|_{g_*=\bar{g}_*}=g_*^{-1}\bar{g}_*\gamma_*(\omega) \tag{19}$$

and similarly for any γ-like function, at any site. A substitution of the atomic GF at a generic site h can also account for the introduction of a local potential v_h at that site. In this case the Hamiltonian (3) would have a further diagonal term $V_{ij}=\delta_{ij}\delta_{ih}v_h$ and the atomic GF would read $\bar{g}_h(\omega)=(\omega-z_h a-v_h)^{-1}$. Now, making use of Eqs. (9) and (13) it is possible to write

$$G_{**}=\frac{g_*}{1-\gamma_*^{\mathcal{B}}-\gamma_*^{\mathcal{T}}}=\frac{g_*}{1-\gamma_*^{\mathcal{B}}}\left[1-g_*^{-1}\left(\frac{g_*}{1-\gamma_*^{\mathcal{B}}}\right)\gamma_*^{\mathcal{T}}\right]^{-1}. \tag{20}$$

When we restrict the structure to $\mathcal{T}$ or $\mathcal{B}$ the GF's at * read, respectively, $G_{**}^{\mathcal{T}}=g_*(1-\gamma_*^{\mathcal{T}})^{-1}$ and $G_{**}^{\mathcal{B}}=g_*(1-\gamma_*^{\mathcal{B}})^{-1}$ Thus, recalling Eq. (19), Eq. (20) becomes

$$\begin{aligned}G_{**}&=G_{**}^{\mathcal{B}}[1-g_*^{-1}G_{**}^{\mathcal{B}}\gamma_*^{\mathcal{T}}]^{-1}\\&=G_{**}^{\mathcal{B}}[1-\gamma_*^{\mathcal{T}}|_{g_*=G_{**}^{\mathcal{B}}}]^{-1}=G_{**}^{\mathcal{T}}|_{g_*=G_{**}^{\mathcal{B}}},\end{aligned} \tag{21}$$

which is nothing but Eq. (17) in the special case $i=*$. The proof for the general case can be obtained in the same fashion. Formula (17) holds for any branching site of the trunk.

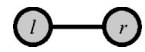

FIG. 2. A dimer.

Thus the GF's at the sites of the trunk can be evaluated by pruning off all the branches, provided that the atomic GF's at the branching sites are changed into the corresponding GF's of the pruned branches. Since they carry all the information relevant to the corresponding branches these new atomic GF's can be viewed as their buds. This operation of bud reduction can be repeated iteratively within the branches and gives rise to a topological simplification of the original structure. Of course for an exact result the knowledge of the exact GF's of the pruned branches is still needed. When these functions are not known a trial expression can be plugged in to get approximate results. From a *down-top* point of view this approach seems well suited for the tailoring of spectral properties. The effect of appending a secondary structure to a known one on the LDOS is simply obtained by plugging in the appropriate atomic GF. Since we will examine only the GF's relevant to the same site, from now on we simplify the notation by dropping one of the repeated subscripts. A superscript will denote the structure relevant to the GF under examination. The following sections contain some examples of bud reduction. We start with very simple building blocks that are then used to deal with more complex structures. The power of bud reduction in dealing with recursively defined structures is illustrated. Since it goes beyond the purpose of the present paper, we refer to a forthcoming article[19] for the detailed discussion of the spectral features.

A. Fundamental building blocks

In this section we apply the technique above illustrated to some simple structures, which can be used as building blocks of more complex networks.

Dimer. A dimer is a simple structure whose graph consists of two sites connected by a link (Fig. 2). Let g_l and g_r be the atomic GF's at its two sites. Since there is only one restricted path starting and ending at either of its sites, it is easy to show that $\gamma_l=\gamma_r=t^2 g_l g_r$. Thus, for a dimer

$$G_l^{\mathrm{d}}(g_l,g_r)=\frac{g_l}{1-t^2 g_l g_r}. \tag{22}$$

Obviously the GF relevant to the other site has the same functional form. It is enough to swap g_l and g_r.

Trimer. A trimer is a simple chain whose graph consists of three sites and two links connecting two external sites to a central one (Fig. 3). Let g_l and g_c and g_r be the atomic GF's at its three sites. Since a trimer can be seen as a dimer branch off-springing from a dimer trunk we can write

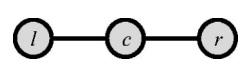

FIG. 3. A trimer.

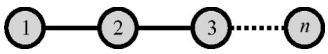

FIG. 4. An *n*-mer.

$$G_l^{\mathrm{t}}(g_l,g_c,g_r)=G_l^{\mathrm{d}}(g_l,G_l^{\mathrm{d}}(g_c,g_r))=\frac{g_l(1-t^2g_cg_r)}{1-t^2g_c(g_l+g_c)},$$

$$G_c^{\mathrm{t}}(g_l,g_c,g_r)=G_r^{\mathrm{d}}(g_l,G_l^{\mathrm{d}}(g_c,g_r))=\frac{g_c}{1-t^2g_c(g_l+g_c)}, \tag{23}$$

$$G_r^{\mathrm{t}}(g_l,g_c,g_r)=G_r^{\mathrm{d}}(G_r^{\mathrm{d}}(g_l,g_c),g_r)=\frac{g_r(1-t^2g_lg_c)}{1-t^2g_c(g_l+g_c)}.$$

n-mer. Iterating the procedure used for the trimer it is possible to deal with a chain of length *n*, for any *n* (Fig. 4). More generally the atomic GF at one end of a *n*-mer can be obtained from the same function relevant to an (k)-mer, $k<n$: $G_1^{(n)}(g_1,\ldots,g_n)=G_1^{(k)}(g_1,\ldots,g_{k-1},G_1^{(n-k+1)}(g_k,\ldots,g_n))$. In particular, when $k=2$

$$G_1^{(n)}(g_1,\ldots,g_n)=G_l^{\mathrm{d}}(g_1,G_1^{(n-1)}(g_2,\ldots,g_n))$$

$$=\frac{g_1}{1-t^2g_1G_1^{(n-1)}(g_2,\ldots,g_n)}. \tag{24}$$

The Green's function at an intermediate site can be obtained by combining the results for dimers and *n*-mers as well: $G_k^{(n)}(g_1,\ldots,g_n)=G_l^{\mathrm{d}}(G_k^{(k)}(g_1,\ldots,g_k),G_1^{(n-k)}(g_{k+1},\ldots,g_n))$, $\forall\, 0<k<n$.

Junction. The central site of a trimer can be seen as a twofold junction joining the two external sites (Fig. 5). A threefold junction can be simply obtained by plugging a dimer GF into the atomic GF of the twofold junction site,

$$G_0^{3\mathrm{j}}(g_0,g_1,g_2,g_3)=G_c^{\mathrm{t}}(g_1,G_{ll}^{\mathrm{d}}(g_0,g_3),g_2)$$

$$=\frac{g_0}{1-t^2g_0(g_1+g_2+g_3)}. \tag{25}$$

The GF at one of the three external sites can be obtained from the one at one end of a dimer by plugging the GF of the central site of a trimer into the atomic GF of the other end,

$$G_1^{3\mathrm{j}}(g_0,g_1,g_2,g_3)=G_l^{\mathrm{d}}(g_1,G_c^{\mathrm{t}}(g_2,g_0,g_3))$$

$$=\frac{[1-t^2g_0(g_2+g_3)]g_1}{1-t^2g_0(g_1+g_2+g_3)}. \tag{26}$$

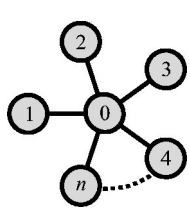

FIG. 5. A junction.

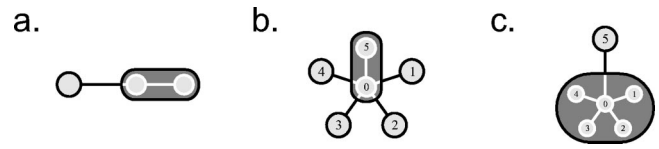

FIG. 6. Examples of simple bud reduction. The dark gray bubbles represent the bud atomic GF's. The white contoured structures inside them are the relevant branches. Note that the new atomic GF are always evaluated at the branching site; (a) Trimer. The two sites on the right site are reduced to a bud. The trimer turns into a dimer. The GF at the left and right site of this dimer give respectively the GF at the left and at the central site of the original trimer; (b) Five-junction. The dimer consisting of the central site and site five is collapsed to its bud. This way it is possible to evaluate the GF's at the origin or at one of the other four peripheral sites by means of the relevant GF's for a four-junction; (c) Five-junction. The four-junction consisting of the origin and of the peripheral sites from one to four is collapsed to its bud. The GF for the dimer allows one to evaluate the GF at site five.

An *n*-fold junction, for any *n*, can be obtained in exactly the same way, simply by iterating the procedure shown above (Fig. 6).

$$G_0^{n\mathrm{j}}(g_0,g_1,\ldots,g_n)=G_0^{(n-1)\mathrm{j}}(G_l^{\mathrm{d}}(g_0,g_n),g_1,\ldots,g_{n-1})$$

$$=\frac{g_0}{1-t^2g_0\sum_{j=1}^{n}g_n}, \tag{27}$$

and

$$G_1^{n\mathrm{j}}(g_0,g_1,\ldots,g_n)=G_l^{\mathrm{d}}(g_1,G^{(n-1)\mathrm{j}}(g_0,g_2,g_3,\ldots,g_n)$$

$$=g_1(1+t^2g_1G_0^{n\mathrm{j}}). \tag{28}$$

B. Infinite Chains

Semi-infinite homogeneous chain (SHC). It is a semi-infinite linear chain with constant atomic GF, *g* (Fig. 7). The GF at its origin can be evaluated by regarding the structure as a SHC branching off from dimer trunk,

$$G_0^{\mathrm{SHC}}(g)=G_l^{\mathrm{d}}[g,G_0^{\mathrm{SHC}}(g)]. \tag{29}$$

Recursion due to periodicity gives rise to a second order equation: $t^2g[G_0^{\mathrm{SHC}}]^2-G_0^{\mathrm{SHC}}+g=0$. The requirement $\lim_{t\to 0}G_0^{\mathrm{SHC}}=g$, Eq. (8), selects the solution,

$$G_0^{\mathrm{SHC}}(g)=\frac{1-\sqrt{1-(2tg)^2}}{2t^2g}=\frac{2g}{1+\sqrt{1-(2tg)^2}}. \tag{30}$$

The GF at a site different from the origin is evaluated as the same function for one of the ends of an *n*-mer, provided that the atomic GF at that end is changed into the GF at the origin of a SHC.

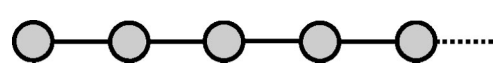

FIG. 7. A semi-infinite homogeneous chain.

FIG. 8. A semi-infinite chain.

Semi-infinite chain (SC). In a semi-infinite chain the origin is a special site; since it is the only site with coordination 1, it may have a different atomic GF (Fig. 8). Let, therefore, g_0 be the atomic GF at the origin and g the atomic GF at any other site.

$$G_0^{\mathrm{SC}}(g_0,g)=G_l^{\mathrm{d}}(g_0,G_0^{\mathrm{SHC}}(g))$$
$$=\left[\frac{1}{g_0}-\frac{1}{2g}(1-\sqrt{1-(2tg)^2})\right]^{-1}. \qquad (31)$$

The procedure for a site different from the origin is the same as the one outlined for the SHC. Both in SC and SHC cases Eq. (31) provides an alternative way: the GF at the kth site is the same as the one for the origin of a SC provided that the atomic GF at the origin is the GF for the end of an appropriate k-mer.

Homogeneous infinite chain (HIC). Let g be the atomic GF at each of the equivalent sites of an infinite chain (Fig. 9). We can obtain the GF at one of these sites by regarding it as a branching site where a SHC branch springs off from a SC trunk.

$$G_0^{\mathrm{HIC}}(g)=G_0^{\mathrm{SC}}(G_0^{\mathrm{SHC}}(g),g)=\frac{g}{\sqrt{1-(2tg)^2}}. \qquad (32)$$

The following bud-reduction schemes yield the same result:

$$G_0^{\mathrm{HIC}}(g)=G_l^{\mathrm{d}}(G_0^{\mathrm{SHC}}(g),G_0^{\mathrm{SHC}}(g))$$
$$=G_c^{\mathrm{t}}(G_0^{\mathrm{SHC}}(g),g,G_0^{\mathrm{SHC}}(g)).$$

Thus Eq. (32) can also be derived from a recursive second-order equation for a trimer. The required GF is the GF at the central site of a trimer in whose external atomic GF's we plug the required result itself. The central atomic GF is the same as in the original structure.

Infinite chain with impurity (ICI). If we change the atomic GF of just one site of the HIC above into g_0 we obtain an infinite chain with a single impurity (Fig. 10). The GF at the impurity site can be obtained by means of the following bud-reduction schemes:

$$G_0^{\mathrm{ICI}}(g_0,g)=G_0^{\mathrm{SC}}(G_0^{\mathrm{SC}}(g_0,g),g)$$
$$=G_l^{\mathrm{d}}(G_0^{\mathrm{SC}}(g_0,g),G_0^{\mathrm{SHC}}(g))$$
$$=G_c^{\mathrm{t}}(G_0^{\mathrm{SHC}}(g),g_0,G_0^{\mathrm{SHC}}(g)),$$

all of which yield

$$G_0^{\mathrm{ICI}}(g_0,g)=\left[\frac{1}{g_0}-\frac{1}{g}(1-\sqrt{1-(2tg)^2})\right]^{-1}. \qquad (33)$$

FIG. 9. A homogeneous infinite chain.

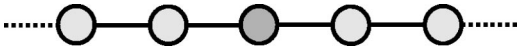

FIG. 10. An infinite chain with impurity.

C. Bethe lattices and Cayley trees

An n-fold Bethe lattice (n-BL) is an infinite network of sites with coordination n, i.e., of n-fold junctions. Note that the HIC is nothing but a 2-BL. Actually a BL is the simplest loopless homogeneous structure after the homogeneous chain. As in a homogeneous chain all the sites of the n-BL are equivalent. For a recent publication on Bethe lattice see Ref. 4. A possible way to work out the GF at one of the n-BL's sites consists in considering any HIC subgraph of this structure as its trunk. Inside each of the n-2 branches offspringing at every site of this trunk one can recognize in turn a SHC trunk, dressed with the same atomic GF as the main trunk. Thus the n-BL can be seen as a HIC, whose atomic GF J is the one for the central site of a (n-2) junction; the atomic GF P for the peripheral sites of this junction are in turn the GF for the origin of a SHC, whose atomic GF's once again equal J. Equation (34) and Fig. 11 display the bud reduction described above:

$$G_i^{n\text{-BL}}=G_0^{\mathrm{HIC}}(J(g)),$$
$$J(g)=G_0^{(n-2)j}(g,\underbrace{S(g),S(g),\ldots}_{n-2\ \text{entries}}), \qquad (34)$$
$$S(g)=G_0^{\mathrm{SHC}}(J(g)).$$

The combination of the last two equations of Eq. (34), together with Eqs. (27) and (30), give a self-consistency equation for J. The GF for the n-BL is thus worked out by plugging the expression obtained for J into Eq. (32), as required by the first of Eq. (34),

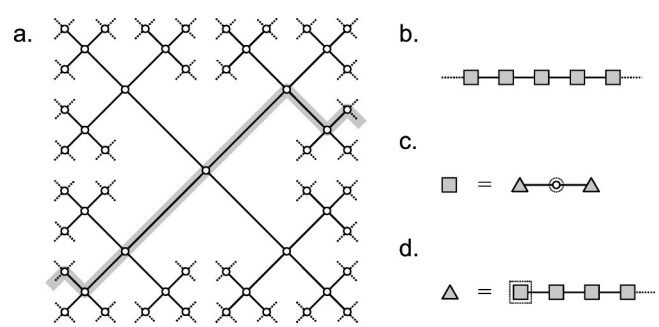

FIG. 11. Four fold Bethe lattice (4-BL); (a) The whole structure is shown. The links are drawn with different lengths just for graphical convenience. The shading shows one possible chain substructure that can be chosen as the trunk for the bud-reduction; (b) Bud-reduced structure: only the trunk is shown. (c) Bud-reduced structure: the structure of the main buds is shown. They consist of trimers whose external sites' GF are the result of a further bud reduction. (d) Bud-reduced structure: the structure of the secondary buds is shown. Note that, due to the recursivity of the structure, they are defined in terms of the main buds. The sites at which the GF's are evaluated are surrounded by dashed lines.

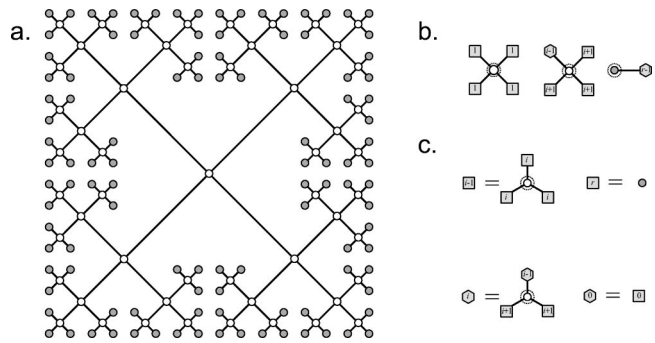

FIG. 12. Fourfold Cayley tree [(4,4)-Ct]; (a) The whole structure is shown. The links are drawn with different lengths for graphical convenience. The sites with coordination $z=1$ are shaded in gray. (b) Bud-reduced structures for the GF of the structure. From left to right: site at the origin, site at distance i from the origin, peripheral site (at distance r from the origin); (c) recursion relations for the bud-reduced structures. The sites at which the GF's are evaluated are surrounded by dashed lines.

$$G_i^{n\text{-BL}}(g)=\frac{2(n-1)g}{n-2+n\sqrt{1-(n-1)(2gt)^2}}. \tag{35}$$

As stated above a Bethe Lattice is an infinite homogeneous structure, and its sites are all equivalent. Its finite version is known as *Cayley tree*.[3] An n-fold Cayley tree of radius r [(n,r) Ct] is a structure invariant under n-fold discrete rotations centered at its central site, which we refer to as its origin. Every site whose distance from the origin is lower than the radius has coordination number $z=n$. The peripheral sites, whose distance from the origin equals the radius, have coordination number $z=1$. A (n,r) Ct is thus a nonhomogeneous structure. Only the sites placed at the same distance from the origin are equivalent. Note that, due to the exponential growth, the number of peripheral sites is of the same order as the number of internal sites. As illustrated by Fig. 12 the GF at the origin of a (n,r) Ct can be obtained by means of three bud-reduction equations,

$$\begin{aligned} G_0^{(n,r)\text{Ct}}(g_i,g_p)&=G_0^{nj}(g_i,\underbrace{L_1(g_i,g_p),\ldots}_{n\ \text{entries}}),\\ L_k(g_i,g_p)&=G_0^{(n-1)j}(g_i,\underbrace{L_{k+1}(g_i,g_p),\ldots}_{n-1\ \text{entries}}),\\ L_r&=g_p, \end{aligned} \tag{36}$$

where g_i is the atomic GF at any of the (equivalent) internal sites, while g_p is the atomic GF at any of the (equivalent) peripheral sites. Note that the second equation of Eq. (36) sets a recursion relation that is closed by the third equation. Also note that imposing the fixed point condition $L_k(g_i)=L_{k+1}(g_i)=L(g_i)$ and plugging the solution into the first equation of Eq. (36) one recovers the result for the n-fold Bethe lattice, formula (35). As illustrated in Fig. 12, the bud reduction for the sites other than the origin is a little more complex, due to the lower degree of symmetry.

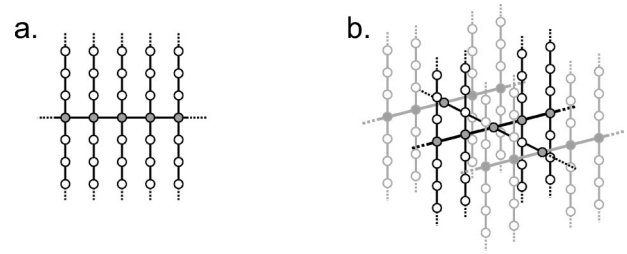

FIG. 13. Fern lattices. Filled circles: sites with $z=4$. Unfilled circles: sites with $z=2$; (a) (2,1) fern lattice, also known as comb lattice or fish bone; (b) (2,2) fern lattice; some secondary structures are drawn in light gray only for graphical convenience.

D. Fern lattices

A fern is a plant characterized by an evident self-similarity. The secondary structures branching off from the the main stalk mimic the whole structure. This resemblance between the branches and the main structure goes on up to a certain order f, at which the branches are simple leaves or stalks. An infinite *fern lattice* (FL) has a similar structure: at every site of an infinite homogeneous chain b identical secondary structures branch off. These are in turn semi-infinite homogeneous chains carrying b identical tertiary structures, and so on. At some order f the b substructures branching off from every site are simple semi-infinite homogeneous chains (see Fig. 13). Thus a fern lattice is characterized by two parameters, the *branching number b* and the *order f*. Most of the sites of a fern lattice, namely, the ones on the branches of highest order, have coordination number $z=2$. All the other ones have coordination number $z=b+2$.

The position of a site relative to the origin of the stalk to which it belongs may be specified by means of two parameters: the distance from the origin and an integer identifying the stalk. This origin is in turn a site belonging to a stalk of lower order, and it may be identified the same way. Thus a site belonging to a secondary stalk of order k ($k=2,\ldots,f$), may be identified by means of $k-1$ pairs of coordinates, plus one more parameter x_1, specifying the coordinate along the main stalk. Due to symmetry properties, sites belonging to stalks of the same order k and identified by the same set of "distance" coordinates, $\{x_2,\ldots,x_k\}$, are equivalent, independent of the remaining coordinates. Thus the GF's at a site belonging to a stalk of order $k>2$, of a (b,f) fern lattice [(b,f)FL] may be identified by means of a vector $\mathbf{x}^{(k)}$ of length $k-1$[$\mathbf{x}_h^{(k)}\geqslant 1 \quad \forall h=1,\ldots,k-1$). The GF at such a site can be obtained as

$$G_{\mathbf{x}^{(k)}}^{(b,f)\text{FL}}(g_s,g_l)=G_{\mathbf{x}_{k-1}^{(k)}}^{\text{SC}}(O_{\mathbf{x}^{(k)}},J(g_s,L_i)), \tag{37}$$

where

$$\begin{aligned} J(g_s,L_i)&=G_0^{bj}(g_s,\underbrace{L_i,L_i,\ldots}_{b\ \text{entries}}),\\ L_i&=G_0^{\text{SHC}}(J(g_s,L_{i+1})),\\ L_f&=G_0^{\text{SHC}}(g_l), \end{aligned} \tag{38}$$

and where g_s is the atomic GF at the sites with coordination number $z=b+2$, whereas g_l is the same quantity for the sites with coordination number $z=2$. The function $O_{\mathbf{x}^{(k)}}(g_s,g_l)$ appearing in Eq. (37) is an appropriate bud-reduced atomic GF, which can be evaluated by a straightforward bud-reduction scheme. Since in the most general case this operation is rather long, we omit it in the present article.

Due to translational invariance the GF's along the main stalk are all equivalent. This makes their evaluation quite easy:

$$G_{\mathrm{ms}}^{(b,f)\mathrm{FL}}(g_s,g_l)=G_0^{\mathrm{HIC}}(J(g_s,L_2)). \tag{39}$$

It is interesting to note that the fixed point relation $L_{i+1}=L_i$ sets in some sense $f=\infty$. In this case all the sites are equivalent and have coordination number $z=b+2$. Thus a n-BL can be thought of as a $(n-2,\infty)$ fern, and indeed Eqs. (38) and (39), together with the fixed point relation, give Eq. (35) once again.

We refer to a forthcoming article[19] for the explicit evaluation of the GF's of some fern lattices of interest.

VI. CONCLUSIONS

In this paper the spectral properties of a single-band tight-binding model applied to inhomogeneous structures are investigated. Since the lack of translational invariance rules out a powerful analytical tool such as the Fourier transform, and forces a direct-space approach, the spectral properties are recovered through the evaluation of the GF's, which are explicitly site-dependent quantities. An analytical technique, based on the properties of the GF's in the presence of branching sites, is developed and illustrated by means of many examples. This technique, which we call bud reduction, allows us to account for an entire substructure off-branching from the network under examination by means of a sort of on-site potential of geometrical origin. It can also be performed telescopically, meaning that the bud-reduced branches may in turn carry substructures which have already undergone bud reduction. This tool yields a topological simplification of the structure under examination and allows a better understanding of the effect of each substructure on the spectral properties of the system. The insight gained on the effects of different topologies may be a guide in designing networks displaying the desired spectral features.

*Email address: buonsant@fis.unipr.it
†Email address: burioni@fis.unipr.it
‡Email address: cassi@fis.unipr.it

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