Tight-binding models on branched structures

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(Received 22 July 1999)

In this paper we analyze the properties of electrons in noncrystalline structures, mathematically described by graphs. We consider a tight-binding model for noninteracting quantum particles and its perturbative expansion in the hopping parameter, which can be mapped into a random-walk problem on the same graph. The model is solved on a wide class of structures, called bundled graphs, which are used as models for the geometrical structure of polymers and are obtained joining to each point of a ''base'' graph a copy of a ''fiber'' graph. The analytical calculation of the Green's functions is obtained through an exact resummation of the perturbative series using graph combinatorial techniques. In particular, our result shows that when the base graph is a *d*-dimensional crystalline lattice, the fibers generate a self-energy of pure geometrical origin in the base Green's functions.

I. INTRODUCTION

The properties of electrons in crystals directly arise from the translation invariance of Bravais lattices through the Bloch theorem. Both the energy spectrum and the eigenstates are described in terms of vectors of the reciprocal lattices and the main mathematical point in this approach is the use of Fourier transform to diagonalize the lattice Hamiltonian. However, most condensed-matter real structures are not crystals and this simple and appealing picture does not apply. This is the case of amorphous materials, glasses, polymers, fractals, and biological systems in general; due to the lack of translation invariance, the Bloch theorem does not hold and the Fourier transform cannot be used as a diagonalization technique. The geometrical complexity can change dramatically the properties of electrons.

The tight-binding model is the simplest description of electrons propagating on discrete structures and very general techniques have been developed to solve the model and to obtain the analytical expression for Green's functions.[1] On noncrystalline structures, where reciprocal space techniques cannot be applied, one has to use direct numerical diagonalization[2] and real-space approaches. In particular, the perturbative expansion in the hopping parameter maps the problem into a walk expansion on the structure, which must be resummed to obtain the exact expression for the Green's function.[3,4] This resummation is nontrivial on noncrystalline structures. As for the analytic approach, on fractal lattices renormalization and decimation techniques can be used due to scale invariance[5] but on general inhomogeneous and disordered networks an alternative method is needed. On a generic graph, this can be found exploiting the graph theoretical formulation of walk statistics which provides very powerful techniques for the calculation of the resummed series. In this paper we will use a generalization of the random-walk approach to analytically solve the tight-binding model for a wide and interesting class of branched networks.

The graph theoretical formulation has been so far successfully applied to vibrational dynamics, diffusion and spin models on general discrete structures, where graphs are introduced to describe the topology of interactions.[6,7] The graphs we will consider here have already been studied from these points of view and they showed very peculiar and interesting properties. They are known as bundled structures and they are obtained through the iterative composition of simpler graphs.[8] For these networks one can introduce an engineering which allows us to build a graph with given properties with the composition of properly chosen structures. Bundled structures are built by connecting a *fiber* graph to each point of a *base* graph and we will see that the presence of the fibers gives rise to a self-energy in the tight-binding Green's functions of the base. This means that the particles moving on the base, though described by a noninteracting Hamiltonian, experience an interaction whose origin is purely geometrical.

II. MODEL

A generic system composed of atoms and electrons jumping from site to site can be described by a quantum Hamiltonian on a graph. A graph is a set of points, representing atoms, connected by links when a nonzero jumping probability for the electrons exists. The free Hamiltonian for an electronic system on a graph can be written by assuming, as usual, the electron motion on the discrete structure to be determined by the overlap between the atomic wave functions of two different sites. In the tight-binding approximation, the superposition between the wave functions ϕ_j and the atomic potentials relative to two different sites are different from zero only if the two sites are connected by a link. The Hamiltonian we obtain is then

$$H = -\sum_{i,j} t_{ij} c_i^\dagger c_j - \sum_i a_i c_i^\dagger c_i , \tag{1}$$

where $c_i^\dagger$ (c_i) is the creation (annihilation) operator of a particle on site i. The parameters t_{ij} and $a_i \equiv \Sigma_l a_{il}$ are given by

$$t_{ij} = -\int d^d r\, \phi_i^*(r)[E_{AT} + V_j(r)]\phi_j(r), \tag{2}$$

$$a_{il} = -\int d^d r |\phi_i(r)|^2 V_l(r), \tag{3}$$

$V_i(r)$ being the potential relative to site i and E_{AT} the atomic energy level. Considering the simplest case $t_{ij} = t$ and $a_{ij} = a$ one obtains for the tight-binding Hamiltonian

$$H = -t\sum_{i,j} A_{ij} c_i^\dagger c_j - a\sum_i z_i c_i^\dagger c_i, \tag{4}$$

where A_{ij} is the (i,j) entry of the adiacency matrix of the graph,

$$A_{ij} = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$

and $z_i = \Sigma_j A_{ij}$ is the coordination number (i.e., the number of nearest neighbors) of site i. When the structure is a regular lattice ($z_i = z$) the local energy term is a constant and one recovers the usual tight-binding model. For a more general structure, z_i varies from site to site and the local term of Eq. (4) must be taken into account.

The solution of the tight-binding model on graphs presents two main problems. First, on a generic graph, due to the lack of translation invariance, the Fourier transform does not diagonalize the adiacency matrix A_{ij} appearing in the hopping term. Moreover, the diagonal terms in Eq. (4), generated by the nonequivalence of graph sites, are nontrivial and their matrix does not commute with A itself.

The perturbative expansion in the hopping parameter t[1] provides a general formal procedure for calculating all Green's functions of the model defined by Eq. (4) on a generic graph: the Green's functions are expressed as a sum over weighted paths, analogous to a path integral. We will briefly recall this expansion in the algebraic graphs theory language.

The Green's functions are defined by

$$G_{ij}(\omega) = -i\int \exp(i\omega t)\langle 0|Tc_i(t)c_j^\dagger(0)|0\rangle dt. \tag{5}$$

Let us start from the ''atomic'' unperturbed Hamiltonian obtained by taking $t = 0$ in Eq. (4). Then the corresponding Green's functions are

$$G_{ij}^{AT}(\omega) = \frac{\delta_{ij}}{\omega + az_i}. \tag{6}$$

Expanding in the hopping term, the tight-binding Green's function can be expressed as

$$G_{ij}(\omega) = \sum_{n=0}^{\infty} (-t)^n G_{ij}^{(n)}(\omega), \tag{7}$$

where the nth-order coefficient $G_{ij}^{(n)}(\omega)$ is the sum over all $n-$steps walks, starting in i and ending in j, of the products of the atomic Green's functions on all sites visited in each walk. Calling $\{\mathcal{W}_n(ij)\}$ the ensemble of all these walks, we have

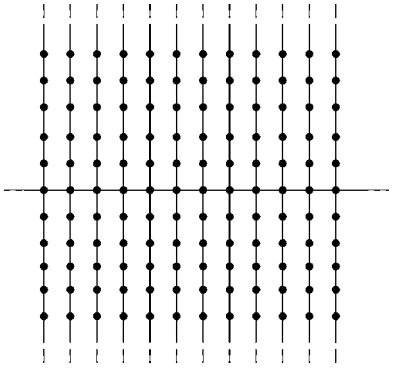

FIG. 1. The comb lattice.

$$G_{ij}^{(n)}(\omega) = \sum_{\{\mathcal{W}_n(ij)\}} \prod_{k \in \mathcal{W}_n(ij)} G_{kk}^{AT}(\omega). \tag{8}$$

The last expression is formally similar to the probability function $P_{ij}(n)$ for a random walk with traps and sources on the graph defined by the jumping probabilities

$$p_{ij} = \frac{A_{ij}}{z_i + d}, \tag{9}$$

where d is the decay parameter, taking into account the effect of traps and sources. Exploiting this similarity we obtain an exact map between the tight-binding Green's functions and the random-walk generating functions $\tilde{P}_{ij}(\lambda) \equiv \Sigma_{n=0}^{\infty} \lambda^n P_{ij}(n)$:

$$G_{ij}(\omega) = \frac{1}{\omega + az_j}\tilde{P}_{ij}(\lambda) \tag{10}$$

with $\lambda = -t/a$ and $d = \omega/a$.

We point out that, in spite of formal similarity, generating functions have very different physical meanings in the above-mentioned problems. Indeed, in random-walk theory they are introduced as a pure computational tool and λ has no physical meaning. As for tight-binding, generating functions have a direct physical interpretation: they are the resummation of the perturbative expansion in the hopping parameter and λ is a function of the parameters appearing in the Hamiltonian.

Now, random walks are one of the most studied physical problems on graphs and analytical techniques are known allowing exact solutions for generating functions on very general families of discrete structures. This is the case for a wide class of graphs called bundled structures, which we will consider in the next section.

III. BUNDLED STRUCTURES

Bundled structures are graphs obtained by joining to each point of a graph called *base* a copy of another graph called *fiber*. A typical bundled structure is the comb lattice showed in Fig. 1, where both base and fiber are linear chains (we shall call them backbone and teeth, respectively). The main random-walks quantities for a generic bundled structure can be related to the corresponding ones for its base and its fiber by analytical techniques.[8] In the following we shall consider only base graphs with constant coordination number.

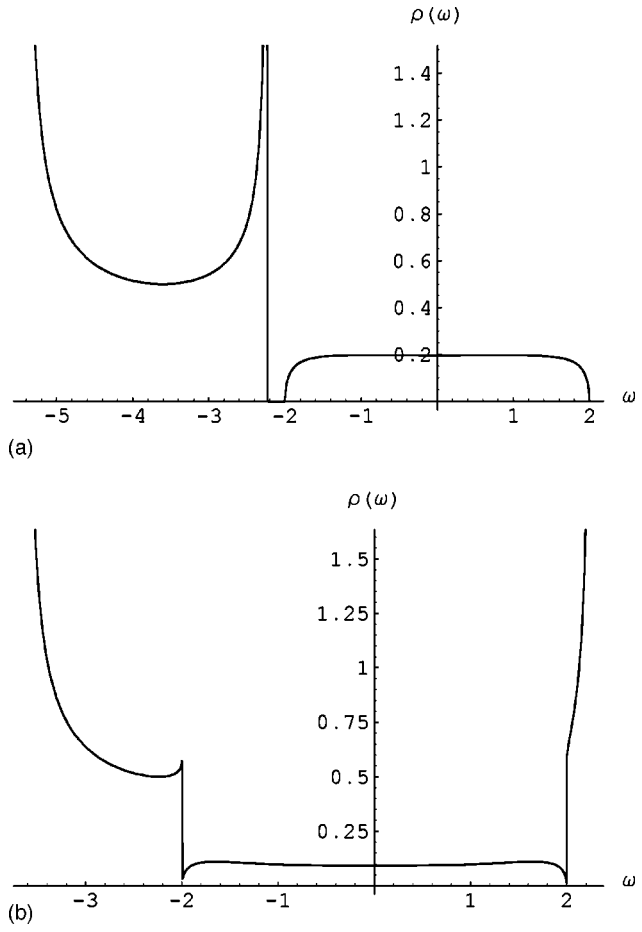

FIG. 2. Local spectral density for the comb lattice, for different values a/t, greater and lower than 1, as discussed in the text: for $a/t>1$ (here we have chosen $a/t=3/2$) there is a gap in the spectral density (a), while if $a/t<1$ (here $a/t=1/2$) the gap closes (b).

We will give the solution of the tight-binding problem on a bundled structure in terms of the solution for the base and the fiber graphs. We call $G_{ii}(\omega)$ and $f_{ii}(\omega)$ the local Green's functions of the base and the fiber, respectively, and we analyze the variation of the local Green's function of the base when it is ''dressed'' by the fibers. Let us consider first the variations of the Green's functions relative to the fibers connected to the base in their origin $i=0$. In this case the coordination number z_0 increases by a quantity that is simply the coordination number of the joining site on the base. It follows that the first effect of the joining is the introduction in the fiber's Hamiltonian of an impurity with energy $-a\Delta z$ and the local Green's function relative to the site $i=0$ becomes[1]

$$F_{00}(\omega)=\frac{1}{a\Delta z+f_{00}^{-1}(\omega)}. \tag{11}$$

Let us now consider the problem of computing the local Green's function for the base. Using the walks statistics for a n-step walk starting and ending at the same base point, we can distinguish between the n_B steps on the base and the $n_F=n-n_B$ steps on the fibers. The n_F steps can also be divided in (n_B+1) groups of steps $n_1,\ldots n_{n_B+1}$. Each group represents the sequence of steps on a fiber between two steps on the base. Notice that some of these groups can also be empty.

Let us call $C_0(n_B)$ the number of n_B-steps closed walk on the base. The nth order of the perturbative expansion in the hopping parameter for the local Green's function relative to one of the base sites is

$$G_{00}^{(n)}(\omega)=\sum_{n_B=0}^{\infty} C_0(n_B)(-t)^{n_B}\sum_{n_1}\cdots\sum_{n_{n_B+1}} F_{00}^{(n_1)}(\omega)\cdots$$
$$\times\cdots F_{00}^{(n_B+1)}(\omega)\,\delta_{n,n_B+\sum_1^{n_B+1} n_i}. \tag{12}$$

Notice that the only constraint on the n_i is that their sum must be n; therefore, after summing over n, all the sums in Eq. (12) become independent. Each sum over n_i gives, by definition, the local Green's function for the fiber with an impurity at the origin, $F_{00}(\omega)$. We then obtain

$$G_{00}(\omega)=\sum_{n_B} C_0(n_B)(-t)^{n_B}[F_{00}(\omega)]^n. \tag{13}$$

Now the perturbative expression (8) when all sites of the graph have the same coordination number is simply given by

$$G_{00}(\omega)=\sum_{n} C_n(-t)^n[G^{AT}(\omega)]^n. \tag{14}$$

Comparing the last two expressions we find the recipe for building the local Green's functions on the base of a bundled structure. Indeed, they can be obtained by replacing in the base Green's function the expression of the atomic Green function with that of the fiber, where the change of z_i in $i=0$ has been taken into account. In this way, attaching a fiber on each site of a graph is equivalent to considering it as composed of ''dressed atoms,'' described by the local Green's function of the fiber.

When the base is translation invariant and the fiber is a generic graph, this ''dressed atom picture'' is more evident. In this case, considering the base's sites only, we can describe the spatial dependence of the Green's functions through the Fourier transform. Since each site of the base is dressed with the same graph fiber, the spatial dependence on the base is the same as that of the undressed base graph. Indicating with $G(\mathbf{k},\omega)$ the Fourier transform of $G_{ij}(\omega)$ $(i,j$ belonging to the base), we get

$$G(\mathbf{k},\omega)=\frac{1}{\omega-\epsilon(\mathbf{k})-\{\omega-[F(\omega)]^{-1}\}}, \tag{15}$$

where $\epsilon(\mathbf{k})$ is the Fourier transform of the hopping matrix on the base. It is clear from expression (15) that the effect of the fiber can be described as a ''self-energy'' in the Green's function on the base. A free model on a bundled structure is equivalent, as far as the base sites Green's functions are taken into account, to a model with an interaction generated by the fiber geometry.

To describe the effects of the ''fibering'' in the bundled structures, we study only local properties. Indeed, all bundled structures in the thermodynamic limit reduce to their fiber graphs and the quantities relative to the ''bulk'' of a

bundled structure coincide with those of the fiber graph.[8] Therefore we will analyze the behavior of the local spectral density on the base:

$$\rho(\omega)=\frac{1}{\pi}\mathrm{sgn}(\omega)\mathrm{Im}[G_{00}(\omega)]. \tag{16}$$

This quantity is commonly used to describe the properties of impurity models, and we expect that it contains most of the information relative to the effects of dressing the base's sites with the fibers.

As an example we present in Fig. 2 the behavior of the local spectral density on the comb lattice, for different values of the ratio a/t. When $a/t>1$, the particle gains in energy if it is delocalized on the backbone only, since the backbone sites have the largest coordination number. The spectral density is composed of two branches, separated by a gap. The first one, whose shape is similar to that of a one-dimensional 1D chain, corresponds to states delocalized on the backbone; the other branch, which is defined for higher values of ω, corresponds to a delocalization on the teeth. On the other hand, when $a/t<1$ the gain in energy if the motion is limited on the backbone sites is not enough and the two branches join. Part of the ''1D-like'' band is shifted to the right of the other branch of the curve. In the ''dressed-atom picture'' we have described above, the motion on the teeth can be interpreted as due to the inner states of the composite base atoms. Therefore the different behaviors of the local density of states describe the energetic competition between these inner states and the Bloch states on the base.

IV. CONCLUSIONS

In this work we used an alternative technique for the calculation of Green's functions of noninteracting quantum particles on noncrystalline structures in the tight-binding approximation, by resumming the perturbative expansion in the hopping parameter. We applied it to a class of branched networks known as bundled structures through exact combinatorial calculations based on random walk statistics. The analytical results show that the geometrical effect of branches is equivalent to the addition of a suitable self-energy on the base structure. This phenomenon suggests that in general the influence of complex geometry on free particles could be viewed as the introduction of a nontrivial interaction in a simpler geometry. We expect to be able to obtain analytic expression for the Green's functions on several classes of graphs by this combinatorial technique applied to the random-walk generating functions. As a final observation, the perturbative expansion in the hopping parameter can also be used for strongly interacting systems with a local interaction, as the Hubbard model.[9] The full knowledge of this graph-theoretical technique in real space on branched graphs represents a first step in the developement of approaches based on hopping expansions for the study of interacting models on inhomogeneous structures.

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