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Renormalization approach for transport and electronic properties of conducting polymers

Riccardo Farchioni and Giuseppe Grosso
Dipartimento di Fisica, Università di Pisa and Istituto Nazionale di Fisica della Materia, piazza Torricelli No. 2, 56126 Pisa, Italy

Giuseppe Pastori Parravicini
Dipartimento di Fisica "A. Volta," Università di Pavia and Istituto Nazionale di Fisica della Materia, via Bassi No. 6,
27100 Pavia, Italy

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By means of the renormalization approach, we have developed a map that allows us to investigate transport and electronic properties in polyaniline chains in terms of an effective lattice. This lattice may contain impurities of two kinds: the first has the form of a couple of sites (dimer) with the same or different site energies according to the symmetry of the rings of the polymer it simulates; the other can occur without constraint in the number of sites involved. In the case of more sophisticated descriptions of the polymer, the dimer model can be inadequate and impurities of four sites have to be introduced in the map. We compare the results for the scattering properties of a single impurity with those of a finite sample of the chain, and we show the dependence of the results on the energies assigned to the carbon and nitrogen atoms of the polymer.

I. INTRODUCTION

The existence of some classes of polymers with surprisingly good conductive properties is presently one of the most interesting topics of condensed-matter physics.[1] A key problem is the explanation of the microscopic mechanism which allows the propagation of electronic waves despite the lack of translational order of the chain.

One of the most significant examples of conducting polymers is constituted by the family of polyanilines, as shown in Fig. 1, whose structure is made by chains of rings of carbon atoms connected by nitrogen atoms. The C atoms nearest to the N atoms are in general indicated as α-C atoms, the other as β-C atoms. The N atoms can exist in a *reduced* form (amine N atoms) or in an *oxidized* form (imine N atoms); if c is the percentage of the oxidized N atoms, the structure of the polymer presents a percentage of $c/2$ rings of quinoid type, i.e., of rings with two C═C bonds. According to the value of c for the oxidation degree of N atoms, we can obtain different parent forms of the polymers: if $c=0$ [*leucoemeraldine* form, fully reduced state; Fig. 1(a)] the chain is entirely composed of benzoid rings. If $c=50\%$ [*emeraldine* form, Fig. 1(b)], there is a fraction of 25% of quinoid rings; if $c=100\%$ [fully oxidized state; *pernigradiline* form, Fig. 1(c)] the quinoid rings are one-half of the total number. Moreover, the amine N atoms can also exist in a protonated form which can be realized, for instance, by means of acidic treatment: the protonated state of the emeraldine is the most conducting parent form.

One of the most significant attempts to understand the conductive properties of polyanilines points attention to the role of a regular sublattice of defects (polarons);[2,3] it is supported by sophisticated investigations of the geometric structure,[4,5] electronic,[2,5,6] and vibrational properties[7] of the polymeric chains. A great impulse to the solution of the problem has been given by introducing the alternative idea to consider as decisive the role of the disorder due to the random distribution of quinoid and benzoid rings in the chain.[8–11] In this approach the system has been generally studied in the frame of the Hückel theory, by assigning to the atoms appropriate site energies and hopping interactions according to the type of bonds. To expect electronic transport in a system dominated by disorder may appear surprising; however, this hypothesis is corroborated by the fact that in certain systems with correlated disorder, or in the presence of internal symmetries of the defects, a part of the eigenstates of the spectrum tends to be delocalized, determining an increase of the conductivity of the system; the simplest form of correlated disorder which is worth mentioning for its consequences on the study of conducting polymers, is the random dimer model;[12–15] it has been deeply studied in the case of binary lattice, but also in more general situations.[16]

The paper is organized as follows: In Sec. II we briefly introduce the renormalization method, which allows us to map the original polymeric chain into an effective one-dimensional lattice. The structure of the map is explained in Sec. III, first for the isolated carbon atom ring, then for the

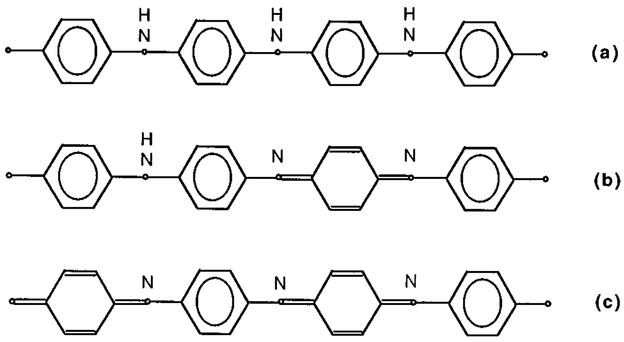

FIG. 1. Scheme of the three principal parent forms of polyanilines: (a) leucoemeraldine (fully reduced form), (b) emeraldine, and (c) pernigradiline (fully oxidized form). Rings with circles inside represent benzoid groups, rings with bars represent quinoid groups.

single quinoid ring embedded in a host regular chain of benzoid rings, and finally for a general distribution of rings. In Secs. IV and V we present results for a single defect ring in a periodic chain, and for a random distribution of rings, respectively. Section VI contains the conclusions.

II. RENORMALIZATION METHOD

In the study of the electronic and transport properties of a polymeric chain, it is convenient to map the complex structure of carbon and nitrogen atoms of the polymer exactly into an equivalent simplified system with the same significant physical properties. For this purpose, the renormalization procedure is a natural choice, because in a simple and natural way it allows us to decimate degrees of freedom of the system and then to calculate the physical quantities of interest (as the Green function) of the remaining effective system.[17] The heart of the renormalization procedure, in the case of a one-dimensional lattice where a_n is the site energies and t_n the hopping interactions, is constituted by the following recursive relations:[18]

$$\varepsilon_0^{(N-1)}(E)=\varepsilon_0^{(N-2)}(E)+t_{0,N-1}^{(\mathrm{eff})}(E)\,\frac{1}{E-\varepsilon_{N-1}^{(N-2)}(E)}\times t_{N-1,0}^{(\mathrm{eff})}(E), \tag{1a}$$

$$\varepsilon_N^{(N-1)}(E)=a_N+t_{N,N-1}\,\frac{1}{E-\varepsilon_{N-1}^{(N-2)}(E)}\,t_{N-1,N}, \tag{1b}$$

$$t_{0,N}^{(\mathrm{eff})}(E)=t_{0,N-1}^{(\mathrm{eff})}(E)\,\frac{1}{E-\varepsilon_{N-1}^{(N-2)}(E)}\,t_{N-1,N}=t_{N,0}^{(\mathrm{eff})}(E). \tag{1c}$$

The above relations provide the effective site energies and hopping interaction of the renormalized system; from them, at the fixed point of the transformations, much information about the electronic structure of the polymer and its transport properties can be obtained. In fact, for instance, the diagonal element $G_{00}(E)$ of the Green function can be obtained from Eq. (1a):

$$G_{00}(E)=\frac{1}{E-\varepsilon_0^{(N)}(E)}$$

(for large N); the poles of G_{00} provide the eigenvalues of the original system, and the residues at the poles the amplitude of the wave function on the site 0; moreover Eq. (1c), through the transfer-matrix formalism, allows us to calculate the transmission (and then the conductivity, by means of the Landauer formula) of a disordered chain embedded in a host periodic lattice.

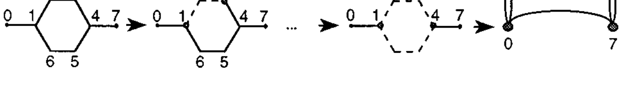

FIG. 2. Steps for the renormalization of a single ring which preserves the nitrogen atoms at sites 0 and 7; carbon atoms from 1 to 6 are decimated. This scheme summarizes the results expressed in Eqs. (2).

In this paper we exploit the renormalization procedure to perform a suitable mapping which allows us in a simple way to investigate the electronic and transport properties of the polyaniline chains and their dependence from the parameters of the Hückel theory (site energies and hopping integrals). As is often done in the literature, we also consider the whole polymer completely lying on a plane (x,y); moreover, the only interactions of interest are due to p_z orbitals.

Once these assumptions are made, the renormalization method reduces the single ring exactly to a diatomic molecule; thus a single quinoid ring embedded in a regular chain of benzoid rings is mapped into a dimer impurity embedded in a regular lattice. In order to perform calculations not only on a single impurity, but also to treat finite samples with an arbitrary number of impurities, we have introduced a map which transforms a general distribution of carbon atom rings separated by nitrogen atoms, into a convenient renormalized lattice. The main effect of the passage from a single impurity to a generic distribution of impurity rings is that the effective renormalized lattice contains random impurities (dimers) with correlated energies, i.e., they occur in the lattice with a probability equal to the concentration of the quinoid rings. The remaining part of the lattice is constituted of sites resulting from the renormalization of at least two consecutive benzoid rings of the chain; a single benzoid ring between two quinoid rings does not appear in the effective renormalized lattice: in fact, as we shall see, its contribution is considered in the site energies of the two consecutive dimers and in the interaction between them. Therefore, these effective sites can have an arbitrary number of occurrences. In the effective lattice there are just two kinds of interactions: (i) interactions internal to the sites of the dimers; and (ii) interactions between two consecutive dimers, between dimers and sites, and between sites, which are all equal. It will be clear that this kind of map automatically excludes forbidden configurations of the chain, as occurrence of two consecutive quinoid rings.[1,2]

III. DESCRIPTION OF THE MAP

Looking at the structure of the simplest form of the polymeric chain [Fig. 1(a)], it can be argued that the renormalization procedure of the single ring can be very conveniently applied by eliminating the C atoms of the rings and preserving the N atoms. Thus we take into consideration the single ring between two nitrogen atoms as the elementary unit to renormalize. The main steps of the procedure for decimating carbon atoms are shown in Fig. 2; after this operation, the ring is reduced to a couple of effective nitrogen atom sites. Here we provide general analytic expressions for the renormalized left and right nitrogen site energies and their interactions which are obtained exploiting Eqs. (1) for an appropriate choice of the Hückel parameters, when the carbon atoms of the ring are decimated:

$$\varepsilon_4=a_0+\frac{t_{01}^2}{E-\alpha-\dfrac{\tau^2}{E-\beta}},\qquad \varepsilon_r=a_7+\frac{t_{47}^2}{E-\beta-\dfrac{\tau^2}{E-\alpha}}, \tag{2a}$$

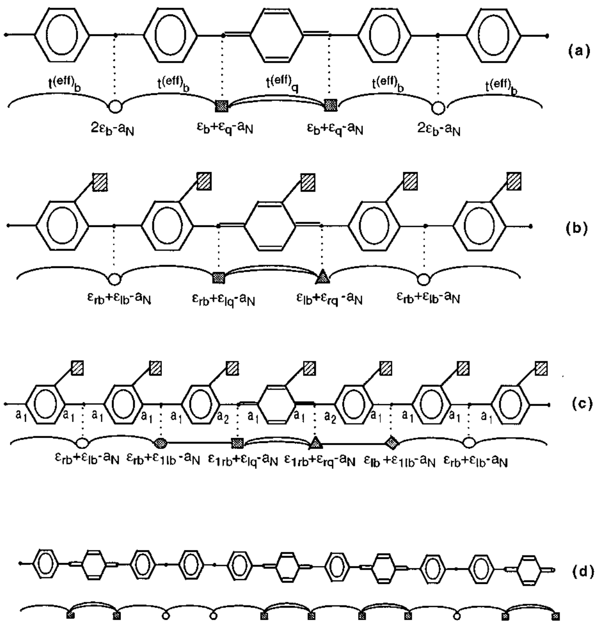

FIG. 3. (a) Map for a chain with a single quinoid ring when the site energies of C atoms are symmetrical with respect to the midpoint between the nitrogen atoms; the impurity is represented by a symmetrical dimer. (b) Map for a chain with a single quinoid ring when the site energies of C atoms are assigned arbitrarily, and the impurity is represented by an asymmetrical dimer. (c) Map for a chain with a single quinoid ring when different site energies of α-C atoms bound to nitrogen amine or imine atoms are assigned. (d) Map for a generic distribution of quinoid and benzoid rings.

$$t^{(\mathrm{eff})} = \frac{t_{01} t_{47} \tau}{(E-\alpha)(E-\beta) - \tau^2}, \tag{2b}$$

where

$$\alpha = a_1 + \frac{t_{12}^2}{E-a_2} + \frac{t_{16}^2}{E-a_6} + \frac{\left(\frac{t_{12}t_{23}}{E-a_2}\right)^2}{E - a_3 - \frac{t_{23}^2}{E-a_2}} + \frac{\left(\frac{t_{16}t_{56}}{E-a_6}\right)^2}{E - a_5 - \frac{t_{56}^2}{E-a_6}},$$

$$\beta = a_4 + \frac{t_{34}^2}{E-a_3} + \frac{t_{45}^2}{E-a_5} + \frac{\left(\frac{t_{23}t_{34}}{E-a_3}\right)^2}{E - a_2 - \frac{t_{23}^2}{E-a_3}} + \frac{\left(\frac{t_{16}t_{56}}{E-a_5}\right)^2}{E - a_6 - \frac{t_{56}^2}{E-a_5}},$$

$$\tau = \frac{t_{12}t_{23}t_{34}}{(E-a_2)(E-a_3) - t_{23}^2} + \frac{t_{16}t_{45}t_{56}}{(E-a_5)(E-a_6) - t_{56}^2}.$$

In these expressions $a_0 = a_7 = a_\mathrm{N}$ are the site energies of the N atoms, $a_1, \ldots, a_6$ are the site energies of the C atoms, and t_{ij} are the hopping interactions. Such quantities, like all the energies in this paper, are expressed in units of $\beta = 2.5$ eV, which is the C-C interaction energy in the aromatic ring.[19] It is not difficult to understand that if the site energies of the ring are assigned with a symmetry with respect to the axes of the N atoms ($a_2 = a_6$ and $a_3 = a_5$, or $a_2 = a_5$ and $a_3 = a_6$ in Fig. 2) the equality $\varepsilon_4 = \varepsilon_r$ holds, and the result of the procedure of renormalization of the ring is a couple of sites with the same effective energy (*symmetric dimer*); otherwise, if no symmetry exists in the ring, the result will be a couple of sites with different energies (*asymmetric dimer*). This symmetry has also a decisive role in deciding the nature of the dimer impurities present in the effective lattice in the case of a general distribution of rings.

After the description of the renormalization procedure in the case of the single ring, we examine the case of single quinoid ring embedded in a host chain of benzoid rings. It is clear that in this case the procedure of renormalization will have to take into account separately the contributions of the rings on the left and right of each N atom. For example, a regular chain of benzoid rings with equal site energies of C atoms will correspond to a regular lattice of N atoms with renormalized site energies $\varepsilon_b = \varepsilon_{rb} + \varepsilon_{4b} - a_\mathrm{N}$ and effective interactions $t_b^{(\mathrm{eff})}$ (the value of the N-atom site energy $a_\mathrm{N} = a_0 = a_7$ has to be subtracted because it is contained both in the expression for ε_4 and in the expression for ε_r; here and in the following the apices b and q indicate the benzoid and quinoid rings, respectively). From the renormalized system the density of states of the original ordered polymeric chain, projected on the N atoms, is immediately available.

In Figs. 3(a)–3(c) the renormalization of the quinoid ring in different situations is presented: in the first case [Fig. 3(a)] the two energies of the dimer are equal because inversion symmetry with respect to the center of the quinoid ring exists; in this case $\varepsilon_{4b} = \varepsilon_{rb} = \varepsilon_b$ and $\varepsilon_{4q} = \varepsilon_{rq} = \varepsilon_q$; the result of the map is a couple of site energies $\varepsilon_b + \varepsilon_q - a_\mathrm{N}$ interacting with $t_q^{(\mathrm{eff})}$, embedded in a host lattice with site energies $2\varepsilon_b - a_\mathrm{N}$ and interaction $t_b^{(\mathrm{eff})}$, which is also the interaction between the impurities and the atoms of the host lattice. Instead, as can be seen from Fig. 3(b) in the case of a single asymmetric quinoid ring (represented with a ring with an external unit linked), the site energies of the dimer are $\varepsilon_{rb} + \varepsilon_{4q} - a_\mathrm{N}$ and $\varepsilon_{4b} + \varepsilon_{rq} - a_\mathrm{N}$, respectively, embedded in a host lattice with site energies $\varepsilon_{4b} + \varepsilon_{rb} - a_\mathrm{N}$; the interactions are the same of the previous case. It has to be observed that the mapping of a single quinoid ring into a dimer is possible if its presence does not influence the two adjacent benzoid rings. If this influence is supposed to be important (for instance, by assigning different values to the site energies of the α-C atoms according to whether they are bound to amine or imine N atoms), those benzoid rings become distinguishable from the other ones of the host lattice; to properly consider this, the quinoid ring plus adjacent benzoid rings are decimated to an effective unit of four sites [Fig. 3(c)].

As a final step, we can now describe the map which transforms a polymeric chain with a general distribution of quinoid and benzoid rings into an equivalent one-dimensional effective lattice; it is based on the renormalization procedure, and is a natural extension of the map for the single ring which has been described above. From Fig. 3(d), it can be seen that each quinoid ring of a polyaniline is mapped into a dimer (for simplicity, we consider the case of symmetric dimers), whose sites are systematically represented with quadrates having site energies $\varepsilon_b+\varepsilon_q-a_{\mathrm{N}}$ and internal interaction $t_q^{(\mathrm{eff})}$. In this map, in general, N benzoid rings are represented by $N-1$ sites of the lattice (circles in the figure) with site energy equal to $2\varepsilon_b-a_{\mathrm{N}}$; their interaction between each other and with the quadrates resulting from the quinoid rings is $t_b^{(\mathrm{eff})}$. It has to be noted that just one benzoid ring between two quinoid rings produces no circle in the effective lattice; its contribution is taken into account in the site energies of the two consecutive quadrates in the lattice, and in the interaction between them. In fact the interaction between adjacent quadrates of two consecutive dimers is $t_b^{(\mathrm{eff})}$. The possibility of two consecutive quinoid rings is automatically forbidden in this kind of map because we avoid the site energy of value $2\varepsilon_q-a_{\mathrm{N}}$.

The procedure of construction of the effective disordered lattice is the following. A random number in the interval [0,1] is generated; if it is less than the concentration of the quinoid rings in the polymer, it is associated with a couple of sites (dimer) with identical energies in the symmetrical case or with different energies for an asymmetrical dimer, and interacting with $t_q^{(\mathrm{eff})}$. Otherwise, it is associated with a single site originated by the renormalization of a benzoid ring, with energy equal to $2\varepsilon_b-a_{\mathrm{N}}$, and the interaction of one site with the following (or between the adjacent sites of two consecutive dimers) is equal to $t_b^{(\mathrm{eff})}$.

In the next two sections, we first analyze the transmission properties of a single defect in an ordered lattice, comparing the results in the cases of symmetrical and asymmetrical dimers and in the case of impurities of four sites; then we analyze the behavior of finite samples with a random distribution of impurity rings.

IV. RESULTS FOR THE EMBEDDED SINGLE IMPURITY

A useful guide to understanding the transmission properties of a finite polymeric chain is the preliminary study of the reflectivity of a single quinoid defect embedded in an ordered chain of benzoid rings; as we have seen before, the related effective system is in general a single impurity with the form of a dimer in an ordered lattice. The dimer is symmetric or asymmetric according to the energies assigned to the C atoms of the ring and to the interactions.

We calculate the reflectivity of the impurity within the energy regions allowed by the host regular polymeric chain. For instance, in Fig. 4(a) we show the reflectivity of the single quinoid ring as a function of the energy calculated in the energy intervals which constitute the spectrum of the periodic host chain of benzoid rings whose total density of states is also represented (dashed lines). As site energies and hopping interactions we have chosen the standard values of Ref. 19. These values are widely adopted in the literature; we have not considered possible improvements of the parameters of Ref. 19, since this paper focuses on the physical origin of the delocalization effects (and does not require to be too specific about the underlying parametrization). As a reference for the energy, here we have considered the simplest case of all carbon site energies of benzoid and quinoid rings equal to zero.

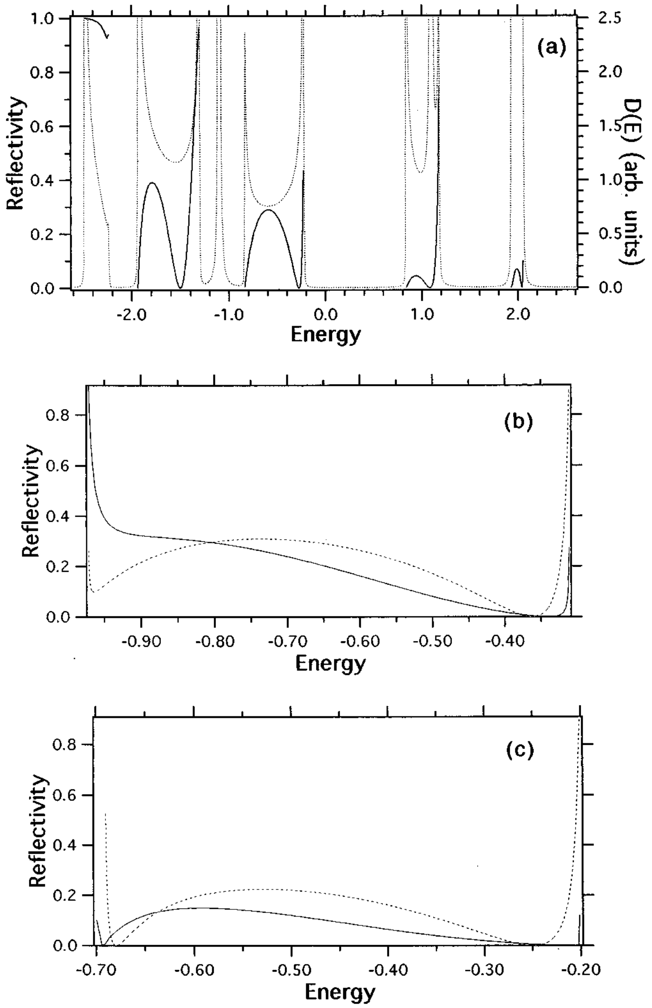

FIG. 4. (a) Reflectivity as a function of the energy of a single quinoid ring with site energies of β-C's equal to zero. The impurity is embedded in a perfect host chain whose density of states is also represented (dashed lines). (b) Reflectivity as a function of the energy of a single quinoid ring when the site energies of β-C's in the ring are equal to zero and the site energies of α-C's have a $a=-0.15$ (dotted line) or have a differentiated correction (full line), i.e., $a=-0.15$ if they are bound to amine nitrogen atoms, and $a=-0.05$ if they are bound to imine atoms (full line). (c) Reflectivity as a function of the energy of a single quinoid ring for site energies of β-C's in the ring equal to zero except $a_3=a_6=+0.5$. The site energies of α-C's have a general correction (dotted line) or a differentiated correction (full line), as in part (a) of the figure.

To examine more realistic examples, corrections to the α carbon atoms site energies may be necessary.[19,20] Now we concentrate on a portion of the energy interval of Fig. 4(a) $(-1\lesssim E\lesssim-0.2)$, because it is the interesting region for conductivity properties of the polymer.[2,3,9] Thus in Fig. 4(b) (dotted line) we report the reflectivity of the dimer as a function of the energy in the case of a general correction of -0.15 to the site energies of the C atoms of type α (bound to N atoms). The site energies of β-C atoms are fixed to zero, the N imine atoms have $a_N=-2$ (we are choosing the case of protonated N imine atoms) and $a_N=-1.5$ for the other N atoms. The hopping between the β-C atoms is -1.1 in the quinoid ring and -1.0 for the benzoid ring; the hopping between α and β-C atoms is always -0.9. It can be observed that there are two minimum points in the reflectivity, which in particular vanishes for $E\sim-0.35$. This value tends to shift, changing the values of the correction for the α-C atoms, reaching the value of $E\sim-0.28$ when no correction is performed. The situation changes if we differentiate the corrections to the site energies of the α-C atoms connected to amine or imine N atoms.[20] In fact, let us consider a correction of -0.15 for the energies of the C atoms connected with amine N atoms, and -0.05 for those connected with imine N atoms; in this case the correct map of the quinoid ring is a four sites impurity [Fig. 3(c)]. We can observe that, even if the overall behavior of the reflectivity is quite different, the reflectivity vanishes again for $E\sim-0.35$ [Fig. 4(b), full line], and the zone of low reflectivity is broader in correspondence to the case of asymmetrical correction.

If we assign the value $+0.5$ to two C atoms of each ring as indicated in Ref. 19, then we have $a_3=a_6=+0.5$ in Eqs. (2). With this assignment of the site energies the properties of a polymer with alkyl groups connected with benzene rings can be described[20] [in this case the poly (2.5-dimethylaniline)]. Here we see that the zones of vanishing reflectivity are two [Fig. 4(c)]: the first is for $E\sim-0.7$, and the second between $E\sim-0.25$ and $E\sim-0.2$, which is again broader in the case of different correction of the site energies of the α-C atoms.

V. CHAINS WITH CORRELATED DISORDER

We have seen in Sec. II that the effective lattice resulting from the map of a polymeric chain of the kinds treated in this paper contains two types of elements: the first is a dimer (or a more complex defect) which can be symmetric, or asymmetric, with internal interaction $t_q^{(\mathrm{eff})}$. The second is a single site which can have an even or odd number of occurrences; the interaction of a single site with the other sites or with the dimers is $t_b^{(\mathrm{eff})}$ [random dimer model[12] (RDM)].

This kind of model is different from the alloy dimer model,[12] where *both* the elements of the lattice can occur only in the form of dimers. The main difference with respect to the alloy dimer model is that, if the dimer is symmetric, just one resonance is present, corresponding to the site energy of the dimer. In general, for an increasing concentration of dimers the width of the interval of good transmittivity of the RDM decreases, up to concentration ~0.9; then the plot of the transmittivity gradually reaches the plot typical of an ordered lattice having the site energies of the dimer and alternating t_q and t_b interactions.

We now examine the transmission properties of some polyaniline chains, from the transmittivity of the equivalent renormalized effective lattice resulting when benzoid and quinoid rings are distributed according to a random sequence. We can see that all the results can be put in correspondence with the results found for the single quinoid ring found in Sec. II; in all cases we have calculated average quantities over 500 generated configurations of effective chains of 1000 sites. All the calculations have been performed following the transfer-matrix approach.[21]

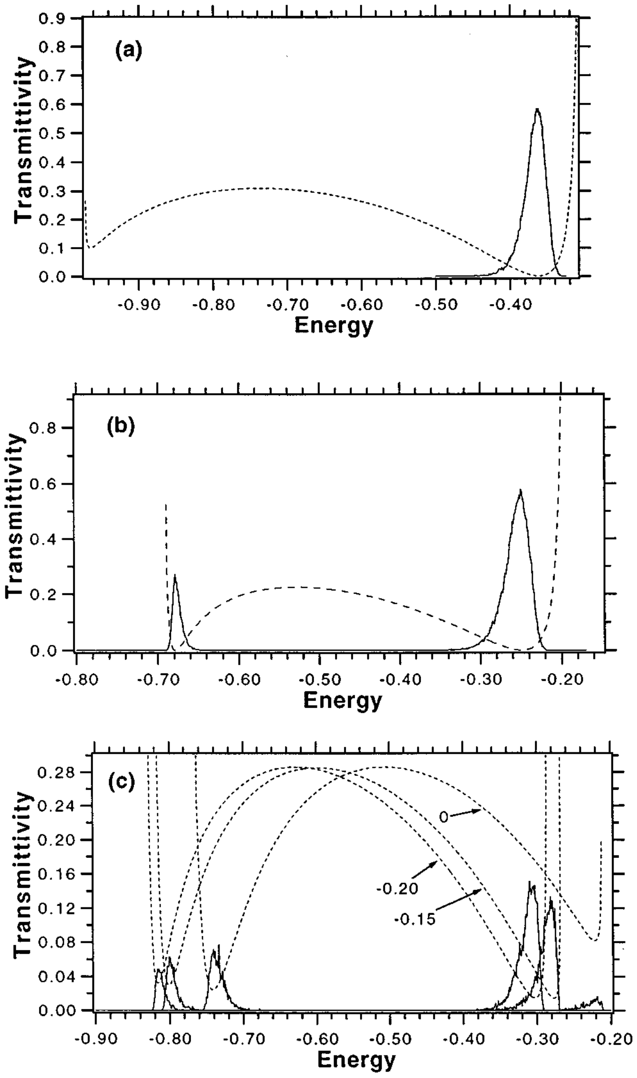

FIG. 5. Transmittivity as a function of energy for two examples of polymeric chains. (a) Case of site energies of β-C's in the rings equal to zero, and site energies of α-C's with a general correction of $a=-0.15$. (b) Case of site energies of β-C's in the rings equal to zero, except $a_3=a_6=+0.5$, corresponding to the polymer poly(2.5-dimethylaniline), and site energies of α-C's with general correction $a=-0.15$. (c) Case of site energies of β-C's in the rings equal to zero except $a_3=+0.5$, corresponding to the polymer poly(*o*-methylanine), when a general correction of 0, -0.15, and -0.2 is given to α-C atoms. In all these cases the length of the samples is $N=1000$, the percentage of quinoid rings is 25%, and the results are averaged over 500 configurations.

The first example concerns the emeraldine parent form of the polyaniline, in its protonated form, where the percentage of quinoid rings is 25%, and a general correction of -0.15 has been given to the α-C site energies. From Fig. 5(a), we see that the sample has an interval of good transmittivity for $E\sim-0.35$; the reflectivity of the single defect is shown for comparison (dotted line), indicating a clear relation between the plots.

The second example of polymer we have examined can be represented, in the Hückel theory, modifying the site energies of two C atoms in each ring according to the prescription $a_3 = a_6 = +0.5$; we remark the fact that the impurity in the form of dimer is again symmetric. The polymer described in this way is the poly(2.5-dimethylaniline), which has the alkyl groups CH and CH_3 linked to the C atoms labeled 3 and 6, respectively, in Fig. 2. We can see from Fig. 5(b) that the two intervals of low reflectivity for the single impurity correspond with two intervals of good transmittivity (averaged over 500 configurations) of the sample. It can be also observed that the transmission is generally higher where the minima of reflectivity are broader.

We conclude our analysis by examining a polymer which is mapped into an effective lattice containing asymmetrical dimers. This is the case of poly(o-methylanine), which can be represented with a group CH_3 linked to atom 3 (see Fig. 2) of the carbon rings. The presence of this radical is taken into account by assigning to a_3 the value $+0.5$,[19] while all the other site energies of C atoms remain fixed to zero. In this case the symmetry described in Sec. II is obviously broken. In Fig. 5(c) are shown the results for this polymer, comparing the cases where the α-C atoms take the values 0, -0.15, and -0.2. It is clear from the plots that in general the asymmetry of the dimer contained in the lattice has the consequence that the reflectivity of the single ring does not reach values as low as in the previous examples, where symmetrical dimers were involved. This fact is reflected, of course, in the transmission of the finite sample in a very detailed way. In fact it can be observed that in general the transmittivity does not reach values higher than 0.2 (to be compared to ~ 0.6 of the previous cases). Moreover, it results clear from the picture that a lower value of the minimum of the reflectivity, and a broader interval around it, causes a general increase of the transmittivity of the sample.

VI. CONCLUSIONS

By the renormalization approach, we have introduced a general procedure to obtain the map of any given planar polymer; it allows us to investigate in a simple way its transport and electronic properties. Comparing the transmission properties of a single impurity and of the model of the lattice which results from the map of some examples of polymeric polyaniline chains, we see that energy intervals of good transmittivity also exist for rather long samples ($N = 1000$). This characteristic becomes more important if symmetry in the site energies of the rings is respected (case of symmetric dimer), but it is also verified for the asymmetric dimer case; this fact can justify the good conductance properties exhibited by this class of polymers. The approach described in this paper can be easily extended to other families of polymeric chains.

ACKNOWLEDGMENTS

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