Numerical investigation of electron localization in polymer chains

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Using finite-size scaling, we have calculated the localization-delocalization phase diagrams for electronic wave functions in different disordered polymeric systems. The disorder considered here simulates finite polymer chain lengths, breaks in the conjugation, and disorder in an external potential. It is shown that a system of interacting chains, even at rather weak interchain interactions, allows for enough flexibility for the scattered waves to avoid dephasing and localization. Localization and the metal-insulator transition in highly conducting polymers are discussed in view of these results. [S0163-1829(98)03604-2]

I. INTRODUCTION

During the past two decades, conjugated polymers have been studied in great detail. From the point of view of physical properties, most interest has concerned their electrical, electronic, and optoelectronic properties. All these properties are based on the process of charge transport in the polymeric material. In particular, as concerns the studies of heavily doped highly conducting polymer samples, the still unanswered question is how these systems can reach a metallic state (high conductivity in the low-temperature limit) and why the conductivity is so high in this state. The metallic state of the conducting polymer is thought to be close to the metal-insulator transition[1] (MIT). Understanding of the MIT in heavily doped conjugated polymeric systems is thus important in order to reach an understanding of how disorder, electron-electron interactions, etc., affect the transport in these systems. Moreover, the weakly interacting chains of the polymeric systems are highly anisotropic. Such systems are also of interest from a more fundamental point of view as an intermediary between the very well studied cases of one and three dimensions.

There are several different conjugated polymers that can be doped to high levels of conductivity. The most well studied is trans-polyacetylene (PA) that upon doping with iodine can reach conductivities up to 10^5 S/cm, comparable to copper. This high conductivity can only be reached in very pure and carefully prepared samples[2,3] and at high doping levels. At these high doping levels, PA shows intrinsic metallic behavior with a nonzero density of states at the Fermi level and a finite resistance in the low-temperature limit.[4] At low and intermediate doping levels ($<7\%$) the conductivity of PA is high at room temperature, but decreases to zero in the low-temperature limit. The charge transport is thermally activated and the material is semiconducting with an energy gap around the Fermi level. In this article we focus on the heavily doped samples and on the disorder driven MIT. This type of study relates closely to experimental studies that show that degradation of the samples as a result of exposure to, for instance, air[5,3] results in the loss of metallic properties.

Disorder in a conducting polymer can be of several different types, e.g., interruption of the chains, variations in torsion angles along the chains, and disorder in the potential from the dopant ions and in the interchain interaction strength. There are different models of structural disorder in heavily doped conjugated polymers. The samples are viewed either as consisting of highly conducting metallic islands with regions of large disorder in between[6] or as an essentially uniform distribution of the disorder.[1] In both these models, the mean free path has to be large, several hundred angstroms or more, in order to explain the large conductivity in the material.

Theoretically, in order to compare with these experimental observations we would like to study the effect of the disorder on the (Anderson) localization of the electronic wave functions. One parameter scaling theory has predicted localization for one- and two-dimensional disordered lattices. In three-dimensional lattices there is a mobility edge that separates localized and extended states in the energy spectrum. Most of the studies of the Anderson model have been numerical[7-10] on cubic lattices with isotropic hopping and randomly chosen on-site energies, but more recently some studies of different anisotropic Hamiltonians[11,12] have been published.

The aim of this study is to get an understanding of the Anderson MIT in an anisotropic model and to understand the effect of disorder on the localization properties of the electronic states at different energies. The studies are performed at different interchain interaction strengths, thereby modeling different degrees of anisotropy. The role of the dimensionality of the sample has been very clearly illustrated by Reghu *et al.*,[13] who showed that it is possible to tune the conducting polymer through the MIT into the metallic regime by applying pressure. The increased interaction between the chains of the polymer with increasing pressure leads to a transition into the metallic state.

The studies are performed using a simple anisotropic tight-binding Hamiltonian. To simulate the interruption of chains we considered the following two models: (i) the on-site energy was raised on randomly chosen sites to create a potential barrier or (ii) the hopping between sites in the chain was decreased. A third type of disorder has also been studied. This disorder has also been studied by several other authors,[11,12] which makes a direct comparison with our results possible: (iii) a random on-site energy. Section II of this article introduces the methodology and some numerical details of the model. Results and discussion are presented in

Sec. III and a summary of our results and conclusions are given in Sec. IV.

II. METHODOLOGY

Conducting polymers are built up from nearly one-dimensional chains packed into a three-dimensional crystalline structure. This type of system can be represented by an anisotropic tight-binding Hamiltonian with larger hopping in the chain direction ($t^\parallel$) than in the perpendicular direction ($t^\perp$). We note in passing that all types of chain structures can be represented by a model of this type. In particular, more complicated polymeric structures than PA can be mapped onto a one-dimensional chain by a renormalization argument.[14]

If we consider only the $2p_z$ orbitals of the polymer chain, we get the one-electron tight-binding Hamiltonian with nearest-neighbor hopping

$$H = \sum_{k,l,m} |k,l,m\rangle \epsilon_{k,l,m} \langle k,l,m| + |k,l,m\rangle t^\parallel_{k,l,m} \langle k+1,l,m|$$
$$+ |k,l,m\rangle t^\perp_{k,l,m} \langle k,l+1,m| + |k,l,m\rangle t^\perp_{k,l,m}$$
$$\times \langle k,l,m+1| + \text{H.c.} \quad (1)$$

The sum is to be taken over a three-dimensional (anisotropic) cubic lattice and $|k,l,m\rangle$ denote the orbitals at the sites along the chains (k) and in a plane perpendicular to the chain axis (l,m). The energy scale is specified by choosing the hopping strength in the k direction to $t^\parallel = -1$ and by setting the on-site energies to $\epsilon = 0$. Hopping in the direction perpendicular to the chain $t^\perp$ is taken to be small, reflecting the anisotropic nature of polymers. Similar types of models have been used in both one-dimensional[15,16] problems and a three-dimensional lattice[17] to describe PA and it is also relevant to other types of polymers as mentioned above. It has also been studied in the context of localization in the layered structure of high-T_C superconductors with on-site disorder by Panagiotides et al.[11] and Zambetaki et al.[12] The values of the hopping chosen to model PA are $t^\parallel = -2.5$ eV and $t^\perp = -0.1$ eV.[1] In units of $t^\parallel$ we get $t^\perp = 0.04$, which is an idealized but realistic approximation for the π-electron band. In order to study the influence of the interchain interaction strength on the localization properties of the wave functions we have also performed calculations for $t^\perp = 0.1$. This value is much to high to describe the polymeric system, but nevertheless gives information about the sensitivity of the system to changes in the interchain interaction strength.

The main drawback of the simple one-particle Hamiltonian in Eq. (1) is that it does not take electron-electron interactions into account, which certainly also are of importance for localization.[18] We also neglect effects of deviations from uniform bond distances. Such deviations are most certainly present even in the highly doped systems and result in pseudogaps around the Fermi energy.[19,20] The effects of such deviations are briefly discussed below, but since the main focus of this work is on the role of the dimensionality, we leave the details of the effects caused by more subtle structural parameters to a future study.[21]

The disorder present in heavily doped conducting polymers can be of various types (see above). Here we focus mostly on the the effect of chain interruptions, including both the effects of sp^3-like defects and the finite length of the chains. Two different types of interruptions have been considered. One is a binary alloy type of disorder in which we set the on-site energy on random sites to a high value $\epsilon = 10$ (in units of $t^\parallel$). These sites create a potential barrier for electrons and thus cause an interruption in the chain. We have also studied interruptions in the chain by setting the hopping along the chain $t^\parallel$ to a small value (0.04) between randomly chosen sites. A third type of disorder is a box distributed on-site disorder with width W where the on-site energies $\epsilon_{k,l,m}$ are randomly assigned between $W/2$ and $-W/2$. This type of disorder has been studied extensively in other types of systems and is included here merely as a reference, even though it has some similarities to disorder caused by irregularities in the potential caused by the dopant ions.

Disordered systems of the type discussed here have successfully been studied by using the transfer matrix method.[9] For a single chain (one-dimensional system), the time-independent Schrödinger equation in the tight-binding approximation can be written $t_n a_{n+1} + (\epsilon_n - E)a_n + t_{n-1}a_{n-1} = 0$, where E is the energy eigenvalue, t_n is the hopping strength between sites, ϵ_n is the on-site energy, and a_n is the amplitude of the wave function at the site n. By iterating this equation we obtain a relation between the amplitudes of the wave function on different sites of the lattice

$$\begin{pmatrix} a_{n+1} \\ a_n \end{pmatrix} = T \begin{pmatrix} a_1 \\ a_0 \end{pmatrix},$$

where $T = \Pi^n_{i=1} T_i$ and

$$T_i = \begin{pmatrix} \dfrac{E - \epsilon_i}{t_i} & \dfrac{-t_{i-1}}{t_i} \\ 1 & 0 \end{pmatrix}.$$

By generalizing this method to a system of coupled chains we consider a bar with a quadratic cross section $M \times M$, where M is the number of chains in each direction perpendicular to the chain axis. For this system of coupled chains we get a transfer matrix that connects the wave function in a slice of the bar with its value on the nearest-neighbor slices in the following way:

$$T_k = \begin{pmatrix} t^{\parallel -1}_k & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} E - H_k & -I \\ I & 0 \end{pmatrix} \begin{pmatrix} I & 0 \\ O & t^\parallel_{k-1} \end{pmatrix}, \quad (2)$$

where $t^\parallel_k$ is the hopping matrix between slice k and $k+1$, H_k is the two-dimensional Hamiltonian of slice k, and E is the energy eigenvalue. The product of transfer matrices gives a connection between the wave function at the two ends of the bar. From this result the transmittance, reflectance, and conductance of the bar can, in principle, be calculated using, e.g., the Landauer formula.[22] However, since the bar is restricted in size in the directions perpendicular to the chain axis, it constitutes effectively a one-dimensional system. When disorder is introduced in such a systems the transmittance is always exponentially decreasing with the length of the bar.[23] The numerical instability given by the exponentially increasing/decreasing eigenvalues of the transfer ma-

trix makes it almost impossible to get correct numerical results for this type of system. To overcome this numerical difficulty we have calculated the Lyapunov characteristic exponents (LCE's) using an orthogonalization procedure described by Benettin and Galgani.[24,9] Still, great care has to be taken to ensure that the results are free from numerical problems. Here we carefully monitor the number of steps between orthogonalization to ensure numerical accuracy. An estimation of the errors in the calculated LCE's was obtained from the standard deviation. This estimate was also used to determine when the LCE's had the required accuracy. A check was made to verify that the pairs of LCE's were equal with opposite sign within three standard deviations. Since this method of calculating the LCE's yields higher accuracy for longer bars, the method can produce results of arbitrary high precision. In practice, however, the accuracy is limited by the computation time and the upper limit is determined by the computational power available.

The localization lengths of the electronic wave functions were calculated as a function of energy and type and strength of the disorder for different widths of the bar from $M = 4$ up to $M = 10$, in some cases up to $M = 16$ (see below). Periodic boundary conditions in the perpendicular direction to the bar were used in all calculations. As discussed above, since M is finite the calculations will result in finite localization lengths when the system was disordered. To determine whether or not the wave functions were localized in the thermodynamic limit a finite-size scaling argument was used. The localization length λ_M and the renormalized localization length $\Lambda_M = \lambda_M / M$ in a bar of cross section $M \times M$ can be calculated from the inverse of the smallest LCE greater than one.[7] The finite-size scaling behavior of the renormalized localization length was studied as a function of the width of the bar. If Λ_M decreases with increasing M, then the wave functions are localized.[7] Correspondingly, the wave functions are extended if Λ_M increases with increasing M. The slope of the renormalized localization length vs M was obtained by a least-squares fit of the results of Λ_M at each value of the energy and disorder.

Calculations were performed on bars with up to 3×10^5 slices (each slice containing $M \times M$ number of sites). The accuracy of the LCE increases with the length of the bar and the calculations were terminated when the standard deviation of the results at each point in the energy vs disorder phase diagram was less than 2%. In some cases the maximum length of the bar was reached before the accuracy had reached 2%, thus producing results with a lower accuracy. However, in all these cases the localization length was large and well into the region of delocalized states. Therefore, we are confident that these less accurate results will not affect the conclusions.

The key assumption behind finite-size scaling is that the localization length of a localized system asymptotically reaches a limiting value as the width of the bar increases, while in the delocalized system the localization length increases linearly with the number of chains in the bar. If the extension of the wave function is smaller than the size of the bar, the boundary conditions and the finite size of the bar should not affect the result when the wave functions are localized. This is indeed the case along the chain direction where we have the possibility to treat lengths of the bar of
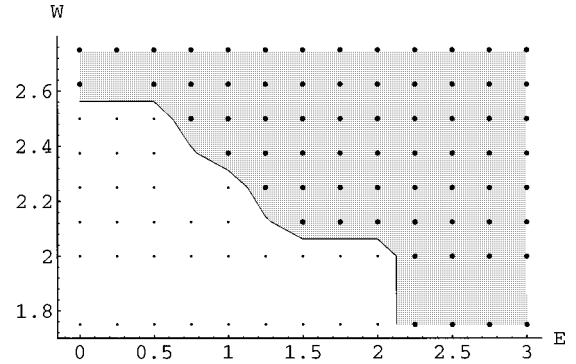

FIG. 1. Phase diagram $t^{\perp} = 0.04$, energy (E) vs disorder strength (W) for box distributed on-site disorder. The dots indicate points that have been calculated. In order to guide the eye, the unshaded area (small dots) shows the parameter space of delocalized states and the shaded area (large dots) the localized states.

the order of 10^5 sites and, as shown below, the localization lengths are up to around 400 sites. The size of the system perpendicular to the chains is, however, much smaller and thus appears to be more critical in this context. Our calculated values of the localization length *along the chain direction* at an interchain hopping strength $t^{\perp} = 0.04$ are $5 - 10$ (depending on the type of disorder) times as large as the size of the bar *perpendicular to the chain axis* for energies and disorder strengths that correspond to states that are on the brink of being delocalized. However, the effect of the disorder is relative to the size of the hopping, so we expect that the localization length in the perpendicular direction should be a lot smaller. From numerical calculations in the case of anisotropic planes with on-site disorder at the center of the band Zambetaki *et al.*[12] have suggested that the following relations holds between the critical renormalized localization lengths parallel and perpendicular to the chain axis: $\Lambda_C^{\perp} = t^{\perp} \Lambda_C^{\parallel}$. In our case, the localization length perpendicular to the chain directions scales down to values that are smaller than M, i.e., the critical renormalized localization length in the perpendicular direction is smaller than one. This indicates that we can extrapolate to the thermodynamic limit and correctly decide whether or not the wave functions are localized. In order to test the effect of using periodic boundary conditions we have performed some calculations with ''hard'' boundary conditions perpendicular to the bar. No change in the behavior of the localization length as compared to the calculations with periodic boundary conditions was observed. This further justifies the use of finite-size scaling in this case.

III. RESULTS AND DISCUSSION

The localization-delocalization phase diagram for the anisotropic three-dimensional (3D) case with on-site disorder is presented in Fig. 1 for $t^{\perp} = 0.04$ and in Fig. 2 for $t^{\perp} = 0.10$. For $t^{\perp} = 0.04$ a disorder of approximately $W = 2$ is needed before the wave functions inside the band start to localize and localization of all states in the band occurs at a disorder strength W of about $2.5 - 2.6$. Decreasing the anisotropy in the system to $t^{\perp} = 0.10$ results in an increase in the the critical disorder to $3.75 - 4.0$. The increase in $t^{\perp}$ corresponds to an increase in the unperturbed bandwidth from 4.32 to 4.8,
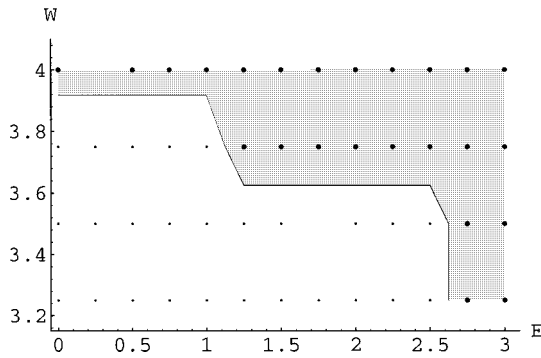
FIG. 2. Same as Fig. 1, but with $t^\perp = 0.10$.

FIG. 4. Phase diagram for $t^\perp = 0.04$, energy (E) vs probability of interruption of chains (P), interruption of chains modeled by setting the hopping between sites in the chains to 0.04 (in units of $t^\parallel$).

thus a relatively small increase showing that it is the hopping strength rather than the total band width that controls the localization properties of the system.

Panagiotides *et al.*[11] derived a relation between the critical disorder (box type) and $t^\perp$. Extrapolating this relation to the values of $t^\perp$ used here, we get a critical disorder of 2.9 in the case of $t^\perp = 0.04$ and 4.0 in the case of $t^\perp = 0.10$, both results in very close agreement with our data.

Our data show clearly the existence of a mobility edge for the anisotropic system with an anisotropy corresponding to that of highly doped conjugated polymers. Thus, from the point of view of transport, the weak hopping that exists between the chains is enough to produce delocalized states even in the presence of relatively strong disorder. The critical disorder for localization of all the wave functions in the band increases with increasing interchain hopping, which is consistent with earlier studies of the same type of system as well as experimental observation of an insulator-to-metal transition driven by applying pressure to the system.[13] For the isotropic system $t^\perp = 1$ the critical disorder is 16.5[8] at an unperturbed bandwidth of 12.0. The behavior of the mobility edge in the anisotropic systems is very similar to the behavior for the isotropic 3D case (see Ref. 10), except that the critical disorder is a lot smaller than in that case.

For the model of chain interruptions involving large on-site energies at certain randomly distributed sites we present a phase diagram (Fig. 3) that shows the region of localized and delocalized states for energies between 0 and 3. The y axis shows the relative concentrations of sites with large on-site energies. As can be seen in Fig. 3, the simple behavior of a single mobility edge that moves towards lower energies with increasing disorder, as in the previous case, disappears. Instead, for a given concentration of defect sites (between
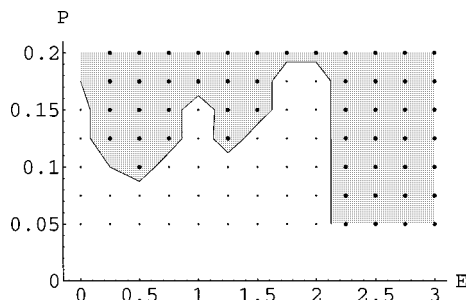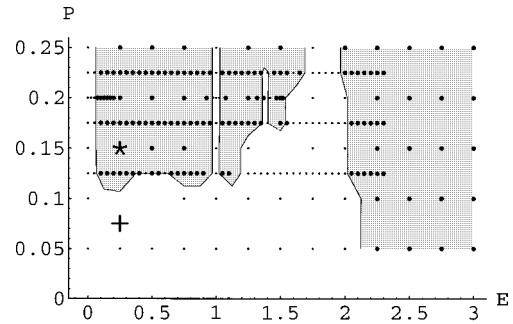

FIG. 3. Phase diagram for $t^\perp = 0.04$, energy (E) vs probability of interruption of chains (P), interruption modeled by setting the on-site energy to 10 (in units of $t^\parallel$).

0.1 and 0.2) several energy regions appear in which the wave functions localize separated by regions of extended wave functions.

The corresponding phase diagram using the second model of chain interruptions with reduced values of $t^\parallel$ between certain randomly chosen sites is shown in Fig. 4. The concentration of such interruptions corresponds directly to the concentration of interruptions caused by raising the site energies. Very interestingly, the two types of defects cause nearly identical phase diagrams. Since we believe that the second model is the most realistic one to describe chain interruption in conjugated polymeric system we have performed a more detailed study of the phase diagram in that case. The small differences between the results presented in Figs. 3 and 4 are caused by the numerical values of the defects and differences in the way these defects scatter the electronic wave function. Our aim of this study is not to make a quantitative comparison between the two types of disorder. However, a rough estimate based on a comparison at a few points in the phase diagram shows that the presently chosen values (see Sec. II above) give very similar localization properties.

For the two types of disorder causing chain interruption it is evident that the critical disorder for localization does not increase monotonically with the energy separation from the band edge; instead there are several mobility edges in this case. The explanation for this phenomenon is that when the interchain hopping is as low as $t^\perp = 0.04$ the chains are very weakly coupled. The interruptions produce short chain segments of varying length. Since the interruptions are randomly generated, approximately half of the chain segments will contain an odd number of sites. The distribution of energy levels for these chains is such that independent on the length of segments, they all produce an energy eigenvalue at zero energy in the limit of noninteracting chains. The accumulated density of states, even in the case of weakly interacting chains, is thus very large at zero energy (see Fig. 5). Furthermore, when adding the energy eigenvalue distribution of all chain segments, we get peaks in the DOS at $E = \pm 1$, $\pm\sqrt{2}, \pm 2\cos(2\pi/5) \approx 0.62\ldots$, simply indicating the density of states (DOS) for chains with specific lengths. To see how well the localization diagram corresponds to the DOS, we have calculated the DOS from the eigenvalues of the Hamiltonian matrix for a system with a length of 40 sites and a 10×10 cross section. The calculations were repeated 16
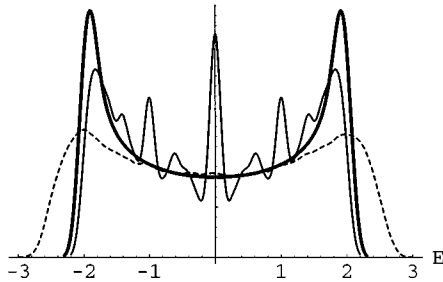
FIG. 5. DOS for $t^\perp = 0.04$: thick solid line, ordered case; solid line, interruptions of chains with low values of hopping between sites ($P = 0.15$); broken line, random on-site disorder ($W = 2.25$).
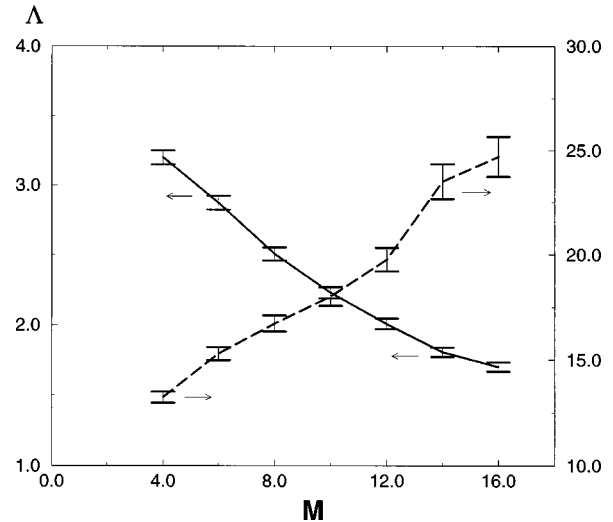

FIG. 6. Renormalized localization length for two points in the phase diagram shown in Fig. 4. The solid and dashed lines correspond to the point marked with * and +, respectively.

times for each type of disorder with different random seeds. The eigenvalues were then used to draw a histogram with intervals of length 0.05; finally the histogram was Gaussian broadened with a width of 0.075. The results for on-site box-type disorder and the chain interruptions by a low value of $t^\parallel$ are shown in Fig. 5. For comparison, the DOS of the perfect lattice calculated from the known energy relation $E_k = \epsilon + 2t^\parallel \cos(k_k) + 2t^\perp [\cos(k_l) + \cos(k_m)]$ is also included in Fig. 5. We also calculated the DOS of a disordered case with breaks in the chains modeled by raising the on-site energy. It shows the same qualitative features as the DOS for the disordered case with interruptions modeled by lowering the hopping, except that it is not completely symmetric around $E = 0$ and additional levels appear at 10 (in units of $t^\parallel$) corresponding to states localized to the defect sites.

Naturally, if the energy levels of two noninteracting chain segments are identical, the electronic states associated with these levels will couple strongly when the interaction between the two chains is turned on. Thus, even though the interchain interaction strength is rather weak, the probability for the electron delocalization is much larger in regions with a high DOS since the closer the energy levels of different orbitals are the greater the chance the electron has to spread. This means that we can explain the increasing transmittance through the sample by having many closely spaced energy levels that in the system of interacting chains increase the probability of the electrons finding a path through the lattice, thereby delocalizing in the thermodynamic limit.

The values of the renormalized localization lengths Λ_M calculated for various sizes of the cross section of the bars (M) at two points in the phase diagram shown in Fig. 4 are shown in Fig. 6. These two points are marked with an asterisk and a plus, respectively, and indicate systems that are in the localized asterisk and delocalized plus regimes, respectively. As is evident from the data shown in Fig. 6, Λ_M is much smaller in the localized regime and reduces with increasing M. In the delocalized regime, however, Λ_M is large and increases with increasing M. We recall from the discussion in Sec. II that this is exactly the signature of delocalization. It is also interesting to note that even though the actual system on which the calculation is performed is finite, the localization length is as large as 400 sites for the bar with the largest cross section ($M = 16$). The bar can be viewed as a fibril in the polymeric system and the result presented here thus gives an indication of the possibility to have very long

mean free paths despite the fact that the system contains a substantial amount of disorder.[25]

Another striking feature of Figs. 1–4 is that, even in regions of low DOS, the phase boundary towards localization appears at a rather high concentration of defects, much higher than what is expected in carefully prepared samples of conjugated polymers. This shows that the anisotropic system is quite robust and that the system can exhibit localization lengths that are much longer than the regions of structural order. This is an important result in connection with the transport properties of, e.g., conjugated polymers.[6]

It should be noted that the situation in the case of conjugated polymers is slightly different from that studied here. The pristine polymer is a Peierls insulator with a gap in the electronic spectrum around zero energy. Upon doping this gap is reduced, and in order for the polymer to exhibit metallic properties, the gap has to be closed. Since this study is more focused on fundamental properties of the anisotropic systems, we avoid effects related to specific models of the metallic state by simply modeling the polymer with uniform bond lengths along the polymer chain.

IV. SUMMARY AND CONCLUSIONS

It is a well known feature of one-dimensional systems that all electronic wave functions become localized in the presence of disorder. Using finite-size scaling, we have shown here that a anisotropic system, even at rather weak interchain interactions, allows for enough flexibility for the scattered waves to avoid dephasing and localization. In heavily doped polymeric material, the Fermi energy lies near the middle of the band. The strength of the disorder that causes localization at these energies is very large, e.g., in the case of $t^\perp = 0.04$ the concentration of chain interruptions needed is around 10% (see Fig. 4), which corresponds to an average chain length of ten CH units. This is clearly an unrealistically small estimate of the chain length. To explain the disorder-induced MIT in heavily doped conjugated polymers one has to con-

sider the effect of residual Peierls distortion (e.g., soliton lattice) to get a more realistic electron structure. Furthermore, it is evident from the evolution of the localization properties with increasing interchain interactions that in order to optimize the transport properties of heavily doped conducting polymers, the interchain interaction is very important.

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