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Effects of doping and interchain interactions on the metal-insulator transition in *trans*-polyacetylene

Magnus Paulsson* and Sven Stafström†
Department of Physics and Measurement Technology, IFM, Linköping University, S-581 83 Linköping, Sweden

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Using a tight-binding Hamiltonian the metal-insulator phase diagram for *trans*-polyacetylene was calculated as a function of doping concentration and interchain interaction strength. The phase boundary for the periodic system coincides with the gap closing, which occurs for certain combinations of critical values for the doping concentration and the interchain interaction strength. The values found are in good agreement with the experimentally observed increase in the Pauli susceptibility. To simulate disorder in the polymer, the effect of finite chain lengths was studied. This type of disorder pushes the metal/insulator phase boundary towards the metallic side of the phase diagram. An increase in the doping concentration and/or interchain interaction is shown to reduce the localizing effects of disorder effectively. For realistic values of the interchain interaction strength the number of chain breaks needed to localize the states at the Fermi energy is quite small, of the order of a few percent. The localization length is found to be substantially longer than the conjugation length of the polymer. [S0163-1829(99)09635-6]

I. INTRODUCTION

The metallic properties of heavily doped conjugated polymers are well documented.[1–6] For *trans*-polyacetylene (PA) there is an onset of the Pauli susceptibility at a doping concentration of 7–8 %, i.e., the density of states (DOS) at the Fermi energy increase rapidly in this regime. However, the transition from nonmetallic to metallic behavior with a non vanishing conductivity at 0 K occurs at a higher doping level since the conductivity is quite sensitive to disorder. Even at the highest doping levels, the metallic samples are close to a disorder-induced transition into a nonmetallic state, as has been demonstrated for instance by applying a strong magnetic field to a metallic sample of poly(*p*-phenylenevinylene) turning it into an insulator.[6] There is an ongoing debate on how the disorder is arranged in the polymers. The homogeneous model,[7] in which the disorder is randomly distributed over the polymer sample and the interesting properties of the conduction is controlled by Anderson localization in the bulk. In the inhomogeneous[8] model the polymer consists of metallic islands with areas of strong disorder in between. This model is more of a percolation transition between nonmetallic and metallic.

Doping of *trans*-polyacetylene is known to create solitons, i.e., kinklike geometrical distortions, along the polymer chains.[9] Each additional dopant charge is associated with one soliton. These distortions align in an ordered way and create a soliton lattice. The electronic structure associated with the soliton lattice consists of a midgap electronic band that is widened with increasing doping concentration, decreasing the size of the bandgap. The soliton lattice can be considered as a Peierls distortion since the length of the unit cell is commensurate with the band filling. For a single chain the Peierls state has a nonzero gap for all doping concentrations and is thus never metallic. Disorder in the polymer will decrease the size of the band gap[10,11] but, in the strictly one-dimensional system, disorder localizes all states[12] however small the disorder is. Thus, both the Peierls effect and the presence of disorder lead to an insulating state in this kind of system.

Electron-electron interactions and lattice fluctuations have been investigated to clarify their effect on the Peierls gap in single chains of PA. The electron-electron interactions, modeled by a Su, Schrieffer, and Heeger (SSH)-extended-Hubbard model reduce the amplitude of the solitons, thus reducing the gap, but do not change the qualitative features of the soliton lattice in PA.[13] The lattice fluctuations, at room temperature, were shown to have an negligible effect on the mean positions of the carbon atoms.[13] Therefore these fluctuations can be considered as an additional source of disorder[14] that, as discussed above, introduce localized states in the band gap.

In order to observe metallic conductivity, i.e., finite conductivity at zero temperature we need to consider three-dimensional effects, here manifested as interchain interactions. The importance of the interchain interactions has been clearly shown in experiments where the polymer is subjected to high pressures, increasing the interchain interaction, causing the samples to make a transition from insulator to the metallic state.[3,5] The Peierls gap will be suppressed by the interchain interaction, since it will widen the electronic bands. Therefore, a gapless state can be obtained even in the presence of a soliton lattice. Furthermore the fact that the polymer chains interact and form a highly anisotropic three-dimensional (3D) system allows for delocalization of the wave function even in the presence of disorder. In an isotropic 3D system, weak disorder will localize states near the band edges but there has to be a large amount of disorder to localize all the states in the band. The size of the disorder required in the isotropic 3D system is demonstrated by the Ioffe-Regel condition,[12] the elastic mean-free path has to be of the order of the lattice parameter in order to localize the wave function. This amount of disorder is not realistic in the polymers discussed here. However, as we have shown in an earlier article,[15] the large anisotropy of the lattice makes it much more sensitive to disorder compared to an isotropic 3D lattice. Based on the previous work one can also expect that states at the Fermi energy will be very sensitive to disorder, especially since the soliton lattice causes a low DOS at the Fermi energy.

In this paper we will show how the interchain interactions close the band gap and how disorder affects both the band gap and the localization properties of *trans*-polyacetylene at various doping concentrations and strength of the interchain hopping. Using a tight-binding Hamiltonian we calculate the band gap of the polymer and in the gapless state the localization properties of the states at the Fermi energy. Due to the complexity of the problem we have been forced to limit the calculations to a one-electron model and limit the possible kinds of disorder to randomly distributed chain breaks. Other types of disorder can of course exist in the polymer samples, lattice fluctuations (as discussed above), the potential from the dopant ions and imperfections in the alignment between chains. The misalignment between chains is particularly important in the model describing the polymeric material as metallic islands separated by regions in which the polymeric chains are more or less randomly oriented with respect to each other. To treat chain misalignment in our model would be to introduce disorder in $t_\perp$ and to effectively reduce this interaction strength. In the presentation below this type of disorder corresponds to the results in the low-$t_\perp$ regime, thus, in an effective way we can also account for this type of disorder in our model.

Section II of this paper introduces the model used to describe PA and the methods used to calculate the band gap and the localization properties of the electronic states. Results and discussion are presented in Sec. III and a summary of the results in Sec. IV.

II. METHODOLOGY

Conducting polymers in the solid state are built up of chains packed into a 3D structure. The electronic properties of this type of system are well described by a simple tight-binding Hamiltonian with large intrachain hopping strength ($t^{\|}$) and a relatively weak hopping perpendicular to the chain direction ($t^{\perp}$). All types of conjugated polymer 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.[16,17] We, therefore, expect that the results that are presented here also give a qualitatively correct picture of localization in other polymers.

Considering the π orbitals of the polymer chain we get the following one-electron tight-binding Hamiltonian with nearest-neighbor hopping only.

$$H=\sum_{k,l,m} |k,l,m\rangle t^{\|}_{k,l,m}\langle k+1,l,m| + \text{H.c.} + |k,l,m\rangle t^{\perp} \times\langle k,l+1,m| + \text{H.c.} + |k,l,m\rangle t^{\perp}\langle k,l,m+1| + \text{H.c.}$$

The sum is to be taken over a 3D cubic lattice, $|k,l,m\rangle$ denote the orbitals at the sites along the chains (k) and in a plane perpendicular to the chain axis (l,m). The anisotropic hopping in the direction perpendicular to the chain, $t^{\perp}$ is treated as a parameter and varied in the range 0.05–0.15 eV including the values that has been suggested for PA.[18]

To take the dimerization of the PA chains into account (as well as soliton defects as described below) the values of the intrachain hopping $t^{\|}$ depends on the C-C bond length. Following Su, Schrieffer, and Heeger[19] (SSH), the hopping strength is approximated as $t^{\|}_{k,l,m}=t_0-\alpha(u_{k+1,l,m}-u_{k,l,m})$ where $u_{k,l,m}$ is the displacement of the k,l,mth carbon atom in the direction parallel to the chain axis. The parameters (t_0, α) were chosen to give a total bandwidth of 10 eV and a band gap of 1.4 eV for a single perfectly dimerized PA chain [$u_k=(-1)^k u_0$], this gives $t_0=-2.5$ eV, $\alpha u_0=-1.4/8$ eV (only the product αu_0 is needed).

In the unperturbed chains the alternating bond lengths of the PA chain were described by $u_k=(-1)^k u_0$ and the geometrical disturbances of the solitons were modeled by setting the displacements of the carbon atoms to

$$u_k=(-1)^k u_0 \prod_n \tanh\left[\frac{k-x_n}{7.0}\right], \tag{1}$$

where x_n is the position of the solitons. This form of the displacements has been shown[20] to correspond very well to the optimized geometry. Each donor/acceptor charge corresponds to one soliton in the lattice, the solitons were placed at fixed distances from each other and from chain ends (defects described below), care was taken to place an even/odd number of solitons on chains with an even/odd number of carbon atoms to ensure that the first and last bond of the carbon chain is a double bond. The doping concentration and thus the soliton concentration will hereafter be denoted y (no. solitons per no. of carbon atoms).

As discussed above the disorder present in heavily doped conducting polymers can be of various types. Here we focus on the effect of conjugation breaking defects such as finite chain lengths, sp^3-hybridized carbon atoms, chain twistings etc. We have simulated these types of defects by setting the hopping along the chain $t^{\|}$ to a small value ($t^{\perp}$) between randomly chosen (adjacent) sites with a given concentration (w). Other types of disorder have not been considered in the calculations, except for a short discussion of the effect of positioning the solitons randomly given in the next section. However, it is our experience that different types of disorder give rise to qualitatively similar results.

The band gap for a 3D crystal without chain breaks and a constant concentration of solitons, perfectly aligned with solitons on the adjacent chains, were calculated from the band structure of a single chain adding the dispersion $2t^{\perp}(\cos[k_y]+\cos[k_z])$ to calculate the 3D band gap. To investigate what effect random alignment of solitons between chains has on the band gap we estimated it from calculations on a finite bar of chains where the chain length was 110 or 111 sites and the bar was composed of 7×7 chains. Periodic boundary conditions were used along the chains and ''hard'' boundary conditions perpendicular to the chains. Averaging the band gap for a large number of random systems (for each y and $t^{\perp}$) and fitting the band gap to a polynomial of $t^{\perp}$ (for each y) enabled us to determine the critical value of $t^{\perp}$ that closes the band gap. The calculations also provided the Fermi-energy for different soliton concentrations, which was used in the calculations of the localization length.

To determine if the electronic states are localized or extended, we use a method developed earlier[15] that treats a system of coupled chains in 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. The product of transfer matrices gives a connection between the wave function at the two ends of the bar. However, this product cannot be used directly to determine whether the wave function is localized or not because of numerical difficulties. Instead, we have calculated the Lyapunov characteristic exponents (LCE) from the transfer matrices using an orthogonalization procedure described by Benettin *et al.*.[21,22] An estimate of the errors in the calculated LCE was obtained from the standard deviation. This estimate was also used to determine when the LCE's had the required accuracy. Since this method of calculating the LCE yields higher accuracy for longer bars, the method can produce results of arbitrary high precision. In practice, however, the size of the system has to be limited due to the extensive computation times. In our calculations for the cases where the states localizes a 1% accuracy was usually met, while for the delocalized cases the accuracy is harder to reach and in most cases the calculation was terminated when the length of the bar reached 3×10^5 sites.

The localization length λ_M, for a bar of cross section $M\times M$, was calculated as the inverse of the smallest positive LCE. From the renormalized localization length $\Lambda_M=\lambda_M/M$ for different sizes M of the bar (with the same defect and soliton concentration) we can determine whether the wave functions are localized or not at the Fermi energy. If the renormalized localization length increases/decreases with increasing width (M) of the bar the states at this energy is delocalized/localized.[23] Using the one parameter scaling hypothesis, we were also able to estimate the localization length of the wave functions in the thermodynamic limit.[22]

III. RESULTS AND DISCUSSION

To investigate how the band gap varies with soliton concentration, interchain interaction strength, and defect concentration we have performed eigenvalue calculations on three cases, without chain breaks with the solitons perfectly aligned between different chains, with randomly aligned solitons and for the disordered case with chain breaks. The phase diagram, showing where the band gap is closed, for the two cases without chain breaks are shown in Fig. 1.

The band gap for the 3D polymer with alignment between solitons on different chains and without chain breaks was calculated for a large number of soliton concentrations (y) and different hopping strength between chains ($t^{\perp}$). The value of $t^{\perp}$ that closes the band-gap, as a function of y, is shown as the solid line in Fig. 1. In the one-dimensional case, i.e., at $t^{\perp}=0$, the system remains insulating for all doping levels due to the Peierls distortion, here present in terms of the soliton lattice. As the interchain interaction is turned on, the Peierls gap is reduced and closed at a certain critical combination of $t^{\perp}$ and y. Increasing y decreases the band gap for a 1D chain and thus lowers the value of $t^{\perp}$ needed to close the gap.

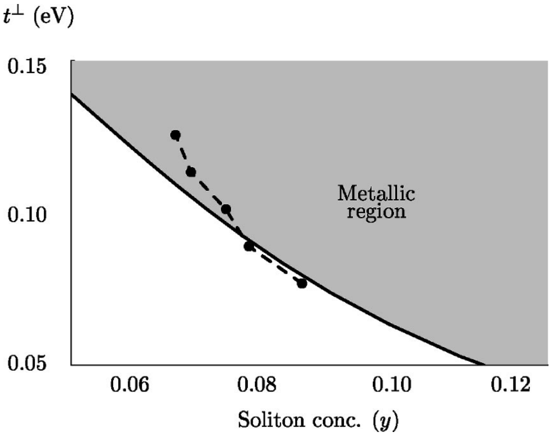

FIG. 1. Phase diagram showing the boundary between the gapless metallic state (top right) and the state with a gap (lower left) for different soliton concentration (y) and coupling between chains ($t^{\perp}$). Solid line shows perfect alignment of solitons between chains; dashed line, random alignment.

To check how random alignment of the solitons between chains and chain breaks change the size of the band-gap, we calculated numerically the eigenvalues of the Hamiltonian for a large lattice. Note that random alignment between solitons on different chains does not affect the ordering of solitons on the individual chains. Averaging over a large number of soliton alignments we were able to estimate the size of the band gap, the Fermi energy and at which soliton concentration the band gap closed for each value of $t^{\perp}$. The perpendicular hopping $t^{\perp}$ needed to close the band gap for the case of no defects and random alignment of the solitons is shown in Fig. 1, dashed line. Compared to the case of perfectly aligned solitons there is no large differences. Thus, at least close to the closing of the band gap, the alignment of the solitons is unimportant as far as the band gap is concerned.

Focusing on the parameter space that is most relevant in the case of *trans*-polyacetylene we note that the experimentally observed rapid onset of the Pauli susceptibility occurs around $y=0.05-0.07$.[24] In the present phase diagram (Fig. 1), this corresponds to an effective interchain hopping of strength of $t^{\perp}=0.10-0.14$ eV, which agrees with the range of values that have been discussed in the literature for the interchain hopping strength.[18]

Defects in materials are known to affect the band gap quite strongly. We have calculated the band gap for disordered finite bars of the same size as used above. Even at as low amounts of chain breaks as $w=1\%$ the band gap closes for all values of $t^{\perp}$ and y that are of practical interest. This fact is consistent with the experimentally measured Pauli susceptibility since the closing of the band gap is caused by the disorder induced tails in the DOS of the soliton and conduction bands. The DOS at the Fermi energy is in this case small since the tails are barely overlapping. These tails are also clearly manifested in optical absorption spectra as a very broad absorption peak associated with the soliton band.[25] The effect on the band gap of random placement of solitons on the individual chains has been studied previously,[10,11] and observed to lead to closing of the band gap as a consequence of disorder, even for a single chain. Thus, even though the ordered system has a band gap the defects inherent in a polymer certainly closes the band gap even at modest amounts of

TABLE I. The critical concentration of chain breaks (w), with error estimates, needed to localize the wave functions at the Fermi energy for different values of $t^{\perp}$ and y. The largest bar cross sections $(M \times M)$ used in the calculations are shown under $M_{\max}$.

$t^{\perp}$ (eV)	y (%)	w (%)	$M_{\max}$
0.075	10	1.5±0.5	10
0.0875	9	1.0±0.5	10
0.0875	10	2.0±0.5	10
0.0875	11	2.5±0.5	10
0.1	8	1.0±0.5	14
0.1	9	2.5±0.5	10
0.1	10	3.5±0.5	14
0.1	11	4.0±0.5	10
0.1	12	4.5±0.5	12
0.1125	9	3.5±0.5	10
0.1125	10	4.5±0.5	10
0.1125	11	5.0±0.5	10
0.125	10	5.5±0.5	10

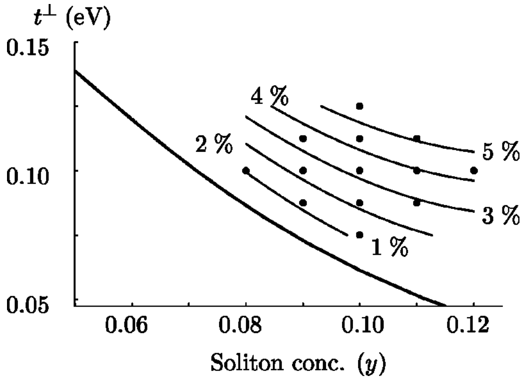

FIG. 2. Schematic metal-insulator phase diagram showing the amount of disorder (w) needed to localize the wave functions for different coupling between chains $(t^{\perp})$ and soliton concentration (y). The contour lines are obtained from data calculated at the marked points. The lower line, taken from Fig. 1 (solid line), shows the closing of the band gap for the ordered case.

doping. However, as shown below, disorder causes localization of the states in the band gap. The transition to a true metallic state in the presence of disorder can only take place at doping levels higher than those corresponding to closing of the band gap for the perfect system (see Fig. 1).

In order to test how sensitive the system of coupled polymer chains is to disorder we have performed calculations of the localization length. Using the concept of finite size scaling we have located the metal-insulator phase boundary as a function of increasing disorder concentration and as a function of $t^{\perp}$ and y. The localization length for bars of polymers (λ_M, where M is the cross section $M \times M$) were calculated for the different values of $t^{\perp}$ and y shown in Table I and for different amounts of chain breaks (w). Since the calculations were carried out on bars (quasi-1D) all states always localize. To extrapolate and answer the question if the states at the Fermi energy are localized in the infinite system we use the finite size scaling argument, the states are localized if the renormalized localization length (λ_M/M) decreases with increasing M. The Fermi energy used was obtained from the band-gap calculations described above, energies close to this energy are also checked to verify that the expected error in the estimated Fermi energy does not significantly change the results.

The metal-insulator phase diagram is shown in Fig. 2. The boundaries between localized (lower left) and delocalized states (upper right) for different amounts of chain breaks are indicated by the lines. The numerical values used to generate the plot were calculated at the points marked in the figure and are listed in Table I.

In the presence of disorder, the randomly distributed chain interruptions can cause localization of the electronic wave functions. In the cases where the band gap has not been closed by interchain interactions disorder move states from the bands into the otherwise forbidden energy gap. Therefore, at the insulating side of the phase boundary in Fig. 1 the gap is reduced and is closed by this effect. However, the disorder-induced tails in the DOS contain localized states. Thus, the parameter space that involve the metallic region is reduced by disorder, as can be seen in Fig. 2.

In Fig. 2, we clearly see that the wave functions localize for small $t^{\perp}$ and y. This reflects that the DOS at the Fermi energy is very important for the delocalization of states. As we have shown earlier,[15] a large DOS makes delocalization easier. For small $t^{\perp}$ and y the DOS at the Fermi energy caused by disorder is small, thereby making localization of the states easy. In contrast, large $t^{\perp}$ and y will remove this pseudogap and the concentration of defects have to be large to localize the states. The experiment by Reghu[3] where samples of heavily iodine-doped PA are shown to cross the metal-insulator transition when pressure is applied to the samples is easily interpreted from Fig. 2. Increasing the pressure will increase the interchain hopping strength causing insulating samples (at normal pressures) to become metallic.

The often used Ioffe-Regel condition states that localization will occur when the inelastic scattering length times the wave vector at the Fermi energy is of the order of one, i.e., the inelastic scattering length is of the order of the lattice parameter. This is clearly a very large amount of disorder, however in the system that we are considering here, localization appear for much lower amounts of disorder. This is clearly an effect of the highly anisotropic structure of the material.[15] The amount of disorder needed to localize the states at the Fermi energy for this model is considerably smaller than for the undimerized system studied previously.[15] In that case the Fermi energy lies in the middle of the conduction band and essentially all states in this band have to localize in order get a transition into an insulating state. The case of the soliton lattice is markedly different in that the Fermi energy lies in the region where the soliton and conduction bands join, as a consequence of the interchain interaction, making the states easier to localize.

The fact that the electronic states localize does not necessarily imply that the transport properties will be dominated by the disorder at all temperatures. At finite temperature the ratio of the elastic to the inelastic scattering length will determine the importance of the disorder.[12] If the inelastic scattering length is short (in comparison with the elastic scattering length) the polymer will behave more as a metal, even though the low temperature behavior is that of an insulator.

The localization length (λ) of the infinite system has been

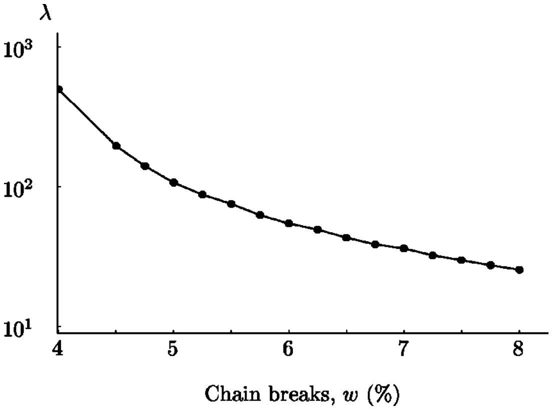

FIG. 3. Localization length λ, logarithmic scale in units of number of carbon atoms, as a function of the amount of disorder. Soliton concentration $y=0.10$, $t^{\perp}=0.1$ (eV).

estimated using the one-parameter scaling hypothesis.[22] To calculate λ we have fitted the localization length (λ_M) for the finite bars with cross section $M\times M$ to the expected $\lambda + c/M$ behavior, for large disorder, where c is a constant. From the calculated localization length for the largest disorder in conjecture with the scaling curve we can estimate the localization length for samples with smaller disorder. The fact that the localization length calculated along the chains of the polymer is larger than the size of the bars (M) used to calculate it, does not imply that the method is questionable since the localization length perpendicular to the chains is approximately a factor $t^{\perp}/t_0$ shorter than the localization length along the chains.[26]

In Fig. 3 is shown the localization length as a function of disorder for systems with $y=0.10$ and $t^{\perp}=0.1$ (eV). The localization length decreases rapidly with increasing w. The mean conjugation length for the chains with disorder is $\sim 1/w$. For all cases shown in Fig. 3, the localization length is more than 2 times $1/w$. This clearly shows the importance of the interchain coupling permitting the wave function to extend past chain breaks.

IV. SUMMARY AND CONCLUSIONS

It is well known that conducting polymers are semiconductors that turn metallic upon large doping. Using a model Hamiltonian for the system of coupled polymer chains we have shown how the band gap in *trans*-polyacetylene (PA) is affected by the doping-induced solitons, interchain interactions and disorder. Our calculations show that the band gap closes at a doping concentration of $\sim 7\%$ for realistic values of the interchain interaction strength in close agreement with the experimentally observed onset of the Pauli susceptibility. Disorder is shown to close the band gap for small amounts of disorder, however the density of states at the Fermi energy is still small. Using finite size scaling, we have calculated the effect of disorder on the electronic wave functions near the Fermi energy. The disorder induced states in the band gap are always localized. Also when the band gap is closed at high doping concentrations the wave functions can be localized by disorder. The amount of chain breaks needed to localize the states at the Fermi energy is quite small as a consequence of the nearly one-dimensional structure of the polymer and the fact that the Fermi energy is located where the soliton and conduction band is joined. We have also shown that the localization length is considerably longer than the conjugation length of the chains, thus the interchain interactions enables the electrons to extend past chain breaks.

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*Electronic address: mpn@ifm.liu.se

†Electronic address: sst@ifm.liu.se

[1] H. Kaneko and T. Ishiguro, Synth. Met. **65**, 141 (1994).

[2] J. Joo, G. Du, V. N. Prigodin, J. Tsukamoto, and A. J. Epstein, Phys. Rev. B **52**, 8060 (1995).

[3] M. Reghu, Synth. Met. **80**, 223 (1996).

[4] M. Ahlskog and M. Reghu, Phys. Status Solidi **205**, 305 (1998).

[5] M. Reghu, C. O. Yoon, D. Moses, Y. Cao, and A. J. Heeger, Synth. Met. **69**, 329 (1995).

[6] M. Ahlskog, M. Reghu, and A. J. Heeger, J. Phys.: Condens. Matter **9**, 4145 (1997).

[7] M. Ahlskog, M. Reghu, A. J. Heeger, T. Noguchi, and T. Ohnishi, Phys. Rev. B **55**, 6777 (1997).

[8] A. J. Epstein *et al.*, Synth. Met. **65**, 149 (1994).

[9] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979).

[10] W. P. Su, Solid State Commun. **47**, 947 (1983).

[11] B. Laks and D. S. Galvão, Phys. Rev. B **56**, 967 (1997).

[12] B. Souillard, *Chance and Matter*, Les Houches Lectures, edited by Jean Souletie, Jean Vannimenus, and Raymond Stora (North-Holland, Amsterdam, 1987), p. 305.

[13] A. Takahashi, Phys. Rev. B **54**, 7965 (1996).

[14] R. H. McKenzie and J. W. Wilkins, Phys. Rev. Lett. **69**, 1085 (1992).

[15] M. Paulsson and S. Stafström, Phys. Rev. B **57**, 2197 (1998).

[16] Y. Chen, S.-J. Xiong, and S. N. Evangelou, J. Phys.: Condens. Matter **9**, 4823 (1997).

[17] R. Farchioni, G. Grosso, and G. P. Parravicini, Phys. Rev. B **53**, 4294 (1996).

[18] M. Reghu, in *Handbook of Organic Conductive Molecules and Polymers*, edited by H. Nalwa (Wiley, West Sussex, England, 1997), Vol. 4, Chap. 2.

[19] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. B **22**, 2099 (1980).

[20] S. Stafström and K. A. Chao, Phys. Rev. B **30**, 2098 (1984).

[21] G. Benettin and L. Galgani, in *Intrinsic Stochasticity in Plasmas*, edited by G. Laval and D. Grésillon (Editions de Physique, Orsay, 1979), p. 93.

[22] A. MacKinnon and B. Kramer, Z. Phys. B **53**, 1 (1983).

[23] J. L. Pichard and G. Sarma, J. Phys. C **14**, L127 (1981).

[24] S. Curran, A. Stark-Hauser, and S. Roth, in *Handbook of Organic Conductive Molecules and Polymers*, (Ref. 18), Vol. 2, p. 34.

[25] A. Feldblum, J. H. Kaufman, S. Etemod, A. J. Heeger, T.-C. Chung, and A. G. MacDiarmid, Phys. Rev. B **26**, 815 (1982).

[26] I. Zambetaki, Q. Li, E. N. Economou, and C. M. Soukoulis, Phys. Rev. Lett. **76**, 3614 (1996).