Localization in quasi-one-dimensional systems

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A general method for obtaining transfer matrices in quasi-one-dimensional systems is presented. We used the method to study Anderson localization in *trans*-polyacetylene, polyparaphenylene, polyparaphenylene-vinylene, and polythiophene. The electron localization length for the polymers as a function of disorder was calculated from the Lyapunov exponents. The polymers are shown to exhibit different sensitivity to disorder, which could be explained in terms of different dimensionality of the polymeric systems. We also give an explanation to the recently observed differences between electron and hole intrachain mobilities in alkoxy derivatives of polyparaphenylene-vinylene, as being a result of the electron-donating nature of the alkoxy substituents.

I. INTRODUCTION

There has been a great interest in the problem of electron localization ever since 1958 when Anderson[1] predicted that all states in a disordered solid should be exponentially localized for a disorder large enough compared to the energy bandwidth. The role of the dimensionality of a system with respect to disorder induced localization is of particular interest. The wave functions in one-dimensional (1D) and 2D systems localize for any[2] nonzero disorder concentration, while for moderate disorder in 3D there is a transition between localized and extended states, where the states in the band tails are localized.[3] Despite being localized, the states in disordered low-dimensional systems are interesting to study in the context of nanoelectronics since the localization length in that case may exceed the size of the sample. Such samples will remain highly conducting even in the presence of disorder.

Numerically, Anderson localization has been studied on systems of all dimensions with particular interest in the scaling behavior of the localization length and the existence of a metal-insulator transition.[4–6] The basic tool in these investigations are the transfer matrices describing the evolution of the wave function as a function of the length of the system. From the transfer matrices the Lyapunov exponents, which render the localization length, can be calculated. Common to all such calculations is that only very simple model systems have been studied, since the construction of the transfer matrices is not straightforward. Typically as a model system one uses a rectangular or cubic array of atoms, which can be subdivided into identical cells. Then *all* atoms in a cell bond to their equivalent atoms in the preceding and succeeding cells, always resulting in a nonsingular matrix describing the intercell interaction. The transfer matrices for systems having a tridiagonal block structure Hamiltonian with nonsingular intercell matrices are readily derived. Using a Green's-function technique a renormalization scheme has been developed to write the transfer matrices of quasi-1D polymers on a form equivalent to that of the simple 1D chain.[7,8] The transfer matrices obtained with this method do, however, describe the evolution of state for only one site per monomer. The connection to the scattering problem has been generally investigated by Molinari.[9] The method of Molinari has recently been used to study transmission in achiral carbon nanotubes, i.e., armchair and zigzag tubes.[10]

Given the transfer matrix many important properties can thus be determined for systems that are too large for the wave functions to be explicitly calculated. There may, however, be restrictions on the type of transfer matrices that can be used, e.g., in calculating the localization length. As will be seen, the transfer matrix for a specific system is most often not uniquely determined though and a suitable matrix has to be constructed. We present in this paper a general method to construct transfer matrices for quasi-1D systems. The method is applied to some common conjugated polymers for which the localization length as a function of random functionalization of a single side group per monomer is calculated. The methodology is introduced and discussed in some detail in Sec. II followed by the presentation of the result in Sec. III. We end the paper with a short discussion concerning both the methodology and the results.

II. METHODOLOGY

A. Transfer matrices

The tight-binding model Hamiltonian can be written as

$$H = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{i \neq j} t_{ij} |i\rangle\langle j|, \quad (1)$$

where ϵ_i is the on-site potential of atom i and t_{ij} is the hopping between atoms i and j. Transfer matrices are usually developed using only nearest-neighbor interaction but may very well incorporate hopping between atoms that are further separated. The simplest case is the 1D chain which has following secular equation relating the coefficients a_i of the wave functions,

$$t_{i-1}a_{i-1} + (\epsilon_i - E)a_i + t_i a_{i+1} = 0, \quad (2)$$

with the hopping t_i in the forward direction. The transfer matrix $\mathcal{T}_i$ is readily derived,

$$\begin{pmatrix} a_{i+1} \\ a_i \end{pmatrix} = \mathcal{T}_i \begin{pmatrix} a_i \\ a_{i-1} \end{pmatrix}, \quad (3)$$

where

$$\mathcal{T}_i = \begin{pmatrix} (E-\epsilon_i)t_i^{-1} & -t_{i-1}t_i^{-1} \\ 1 & 0 \end{pmatrix}. \tag{4}$$

In the more general case of a quasi-1-D system the cells consist of M atoms. The restriction is that atoms in cell i only couple to atoms in cells $i\pm1$. The Hamiltonian will then be block tridiagonal. The secular equations can be written in block form, using the symmetry of the Hamiltonian,

$$\mathbf{T}_{i-1}^\dagger \mathbf{A}_{i-1} + (\mathbf{H}_i - E\mathbf{I})\mathbf{A}_i + \mathbf{T}_i \mathbf{A}_{i+1} = \mathbf{0}, \tag{5}$$

where $\mathbf{A}_i$ is a vector containing M coefficients. The on-site potentials and hopping within cell i is described by the symmetric $M\times M$ matrix $\mathbf{H}_i$, and the coupling to the neighboring cells by $M\times M$ matrices $\mathbf{T}_{i-1}^\dagger$ and $\mathbf{T}_i$. $\mathbf{I}$ is the identity matrix. It is, however, not straightforward to obtain the transfer matrix from Eq. (5) since the $\mathbf{T}$ matrices in general are singular. We show below how this apparent problem in many cases can be overcome. By multiplying two consecutive secular matrix equations by the $M\times M$ matrices $\mathbf{X}_{i1}$ and $\mathbf{X}_{i2}$, respectively, we get

$$\mathbf{X}_{i1}\mathbf{T}_{i-1}^\dagger \mathbf{A}_{i-1} + \mathbf{X}_{i1}\hat{\mathbf{H}}_i \mathbf{A}_i + \mathbf{X}_{i1}\mathbf{T}_i \mathbf{A}_{i+1} = \mathbf{0}, \tag{6}$$

$$\mathbf{X}_{i2}\mathbf{T}_i^\dagger \mathbf{A}_i + \mathbf{X}_{i2}\hat{\mathbf{H}}_{i+1}\mathbf{A}_{i+1} + \mathbf{X}_{i2}\mathbf{T}_{i+1}\mathbf{A}_{i+2} = \mathbf{0} \tag{7}$$

with the notation $\hat{\mathbf{H}}_i = \mathbf{H}_i - E\mathbf{I}$. Combining Eqs. (6) and (7), writing $\mathbf{X}_i = (\mathbf{X}_{i1}\ \ \mathbf{X}_{i2})$ then gives

$$\mathbf{X}_i \begin{pmatrix} \mathbf{T}_{i-1}^\dagger \\ \mathbf{0} \end{pmatrix}\mathbf{A}_{i-1} + \mathbf{X}_i \begin{pmatrix} \hat{\mathbf{H}}_i \\ \mathbf{T}_i^\dagger \end{pmatrix}\mathbf{A}_i + \mathbf{X}_i \begin{pmatrix} \mathbf{T}_i \\ \hat{\mathbf{H}}_{i+1} \end{pmatrix}\mathbf{A}_{i+1}$$
$$+ \mathbf{X}_i \begin{pmatrix} \mathbf{0} \\ \mathbf{T}_{i+1} \end{pmatrix}\mathbf{A}_{i+2} = \mathbf{0}. \tag{8}$$

If $\mathbf{X}_i$ is chosen so that

$$\mathbf{X}_i \begin{pmatrix} \mathbf{T}_i & \mathbf{0} \\ \hat{\mathbf{H}}_{i+1} & \mathbf{T}_{i+1} \end{pmatrix} = (\mathbf{I}\ \ \mathbf{0}), \tag{9}$$

then

$$\mathbf{A}_{i+1} = -\mathbf{X}_i \begin{pmatrix} \hat{\mathbf{H}}_i \\ \mathbf{T}_i^\dagger \end{pmatrix}\mathbf{A}_i - \mathbf{X}_i \begin{pmatrix} \mathbf{T}_{i-1}^\dagger \\ \mathbf{0} \end{pmatrix}\mathbf{A}_{i-1} \tag{10}$$

and the transfer matrix can be constructed in the same way as in Eq. (3). Note that the only assumption made about the system is the tridiagonal-block structure of its Hamiltonian. The internal structure of the cells may be varying as well as the hopping values. Equation (9) may be rewritten in the more familiar form $\mathbf{CX} = \mathbf{D}$:

$$\begin{pmatrix} \mathbf{T}_i^\dagger & \hat{\mathbf{H}}_{i+1} \\ \mathbf{0} & \mathbf{T}_{i+1}^\dagger \end{pmatrix}\mathbf{X}_i^\dagger = \begin{pmatrix} \mathbf{I} \\ \mathbf{0} \end{pmatrix}. \tag{11}$$

A unique solution to Eq. (11) exists only when the $2M \times 2M$ $\mathbf{C}$ matrix has a nonzero determinant. This is often not the case and there may then be either no solution or infinitely many. The criterion for the existence of a solution is that every column in $\mathbf{D}$ is a linear combination of the columns in $\mathbf{C}$. This also implies that the transfer matrix in general is not uniquely determined.

In general, $\mathbf{C}$ will be rank deficient and from the infinite set of solutions (if they exist) to Eq. (11), the minimum norm solution ($\|\mathbf{Cx} = \mathbf{d}\|_2 = \min$; $\mathbf{x}$ and $\mathbf{d}$ are column vectors in $\mathbf{X}$ and $\mathbf{D}$) can be obtained from, e.g., singular value decomposition (SVD) or complete orthogonal factorization.[11] Any other solution can then be acquired from the null space vectors of Eq. (11). However, we emphasize that the existence of a solution to Eq. (11) may depend on the choice of cell structure.

B. Lyapunov exponents

The evolution of a state can be described by the product of transfer matrices $\mathcal{T}_i$,

$$\mathbf{Q}_n = \prod_{i=1}^{n} \mathcal{T}_i. \tag{12}$$

If the determinant of every $\mathcal{T}_i$ is finite and nonzero it follows from a theorem of Oseledec[12] that the following limiting matrix exists

$$\mathbf{\Gamma} = \lim_{n\to\infty} (\mathbf{Q}_n^\dagger \mathbf{Q}_n)^{1/2n}. \tag{13}$$

$\mathbf{\Gamma}$ has eigenvalues $\exp(\gamma_j)$, where γ_j denotes the Lyapunov characteristic exponents (LCE's) of $\mathbf{Q}$. The LCE's may be identified with the rate of exponential decay of the wave functions, where the smallest[13] exponent corresponds to the longest decay length and hence the localization length of the system.[6] The localization length λ is then taken as the inverse of the smallest LCE.[4] Since the eigenvalues of $\mathbf{\Gamma}$ may differ by several orders of magnitude, numerical difficulties often arise in determining the smallest LCE. This problem can be overcome by using an orthogonalization process suggested by Benettin and Galgani.[14]

For the special case when $\mathbf{Q}_n$ is symplectic the Lyapunov exponents will occur in pairs whose elements are the inverse of each other and it is sufficient to determine only the *positive* half of the exponents. For a 2×2 matrix $\mathbf{Q}$ this holds if $\det \mathbf{Q} = 1$, and the reciprocity of the Lyapunov exponents is then very helpful in estimating the numerical discrepancies. In the calculations presented in Sec. III the relative error between the absolute values of the reciprocal exponents was used as a convergence criterion. A relative error of less than 1% indicated a satisfactory convergence and increasing the number of matrix products by a factor of 10 did not significantly alter the result. Typically, 5×10^7 matrix products were used to calculate the largest localization lengths.

III. RESULTS

The transfer matrices of *trans*-polyacetylene (PA), polyparaphenylene (PPP), polyparaphenylene-vinylene (PPV), and polythiophene (PT) have been constructed using the tight-binding Hamiltonian. Equation (11) was solved analytically for computational efficiency as well as to avoid numerical divergence. The repeating cells were chosen according to Fig. 1. With this choice, for all polymers, a 2×2-transfer matrix describing the evolution of state for the two last sites in each cell could be derived. All wave-function coefficients in a cell were described by linear combinations of these two
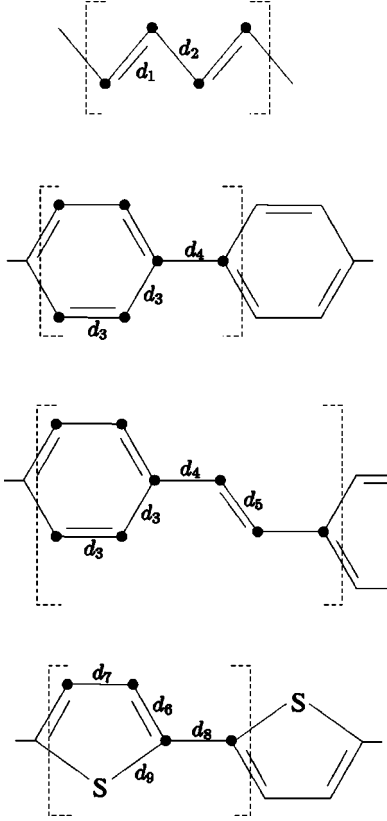
FIG. 1. The carbon backbones for PA, PPP, PPV, and PT, indicating the chosen cell structures for the transfer matrices. The distances referred to are listed in Table I.

FIG. 2. The maximum localization length λ_{max} vs disorder strength W for both undimerized (filled symbols) and dimerized (hollow symbols) PA (triangles) and PPP (circles). W is given in units of the hopping.

last sites of the preceding cell. Hence the exponential decay of any wave function of the above polymers is assessed through these transfer matrices. Moreover, their determinants are always equal to 1.

For the special case of PA a 2×2-transfer matrix with determinant equal to 1 can also be constructed using a cell consisting of only one atom. This follows from a factorization of Eq. (3):

$$\mathcal{T}_i = \begin{pmatrix} (E-\epsilon_i)t_i^{-1} & -t_{i-1}t_i^{-1} \\ 1 & 0 \end{pmatrix}$$
$$= \begin{pmatrix} t_i^{-1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} E-\epsilon_i & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & t_{i-1} \end{pmatrix}. \quad (14)$$

Upon multiplying several such matrices the factors can be grouped together resulting in an effective transfer matrix[15] S_i with the desired properties:

$$S_i = \begin{pmatrix} E-\epsilon_i & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & t_{i-1} \end{pmatrix} \begin{pmatrix} t_{i+1}^{-1} & 0 \\ 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} (E-\epsilon_i)t_{i+1}^{-1} & -t_{i-1} \\ t_{i+1} & 0 \end{pmatrix}. \quad (15)$$

Such an approach has been used for studying the metal-insulator transition in bulk PA taking interchain interactions into account.[16]

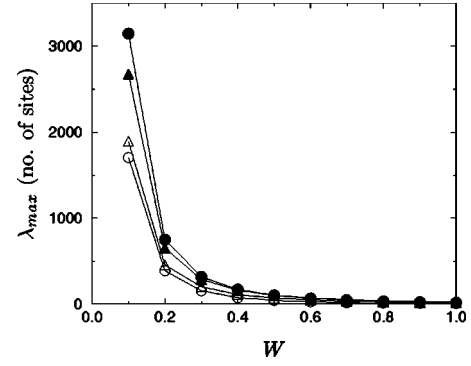We have studied Anderson localization arising from on-site disorder, keeping the hopping fixed. A comparison of the localization lengths in PA and PPP using random on-site potentials with a rectangular distribution $\alpha \in [-W,W]$ and the hopping set equal to 1 (no dimerization) was made. The localization lengths were calculated for different energies E, and the maximum localization length λ_{max} is shown in Fig. 2 as a function of W for both polymers. The value of λ is always given in units of the number of atom sites spanned in the direction of the polymer, e.g., with the cell choice of Fig. 1, PPP has four such sites per cell and PPV six.

The maximum localization lengths are found close to the band gap for both polymers. From Fig. 2 we see that these states are slightly more extended in PPP than in PA. Even though the energy bands of PPP are more narrow than the single band of undimerized PA, the former polymer seems, however, more insensitive to disorder than the latter from a delocalization point of view. This may be attributed to the higher dimensionality of PPP compared to PA. With this we mean that there are more alternate routes combining two transversely separated points, per unit length, in PPP than in PA.

The situation is changed when dimerization of the polymers is considered. The difference in bond length within the polymers can be accounted for using the following relation for the hopping parameters:

$$t = -t_0 e^{-(r-R_0)/\zeta} \quad (16)$$

with r being the interatomic distance. Here the parameters $t_0 = 2.5$ eV, $R_0 = 1.40$ Å, and $\zeta = 0.284$ Å^{-1} were chosen to give a total bandwidth of 10 eV and a band gap of 1.4 eV for a single dimerized *trans*-polyacetylene chain,[16] at a bond-length alternation of 0.8 Å. From now on all the energies will be given in units of t_0.

With this parametrization, the hopping corresponding to the different bond lengths in Fig. 1 were determined; see Table I. The on-site potentials for undisturbed carbon atoms were set to zero and for sulfur[20] -1.33 t_0. The maximum localization length for dimerized PA and PPP with the rectangular disorder distribution is shown in Fig. 2. In this case PA has slightly longer localization length, which can be explained by the fact that the interring distance in PPP is considerably longer than any bond length in PA. This relatively weak bond in PPP leads to smaller bandwidths and a higher sensitivity to disorder. One should be cautious comparing the

TABLE I. The interatomic distances and corresponding values of the hopping [from Eq. (16)] for the polymer structures as indicated in Fig. 1. The energies are given in units of t_0 (= 2.5 eV).

PA [a] :	$d_1 = 1.36$ Å	:	$t_1 = -1.15$
	$d_2 = 1.44$ Å	:	$t_2 = -0.87$
PPP [b] :	$d_3 = 1.41$ Å	:	$t_3 = -0.97$
	$d_4 = 1.51$ Å	:	$t_4 = -0.68$
PPV [c] :	$d_3 = 1.41$ Å	:	$t_3 = -0.97$
	$d_4 = 1.51$ Å	:	$t_4 = -0.68$
	$d_5 = 1.35$ Å	:	$t_4 = -1.19$
PT [d] :	$d_6 = 1.36$ Å	:	$t_6 = -1.15$
	$d_7 = 1.43$ Å	:	$t_7 = -0.90$
	$d_8 = 1.48$ Å	:	$t_8 = -0.75$
	$d_9 = 1.75$ Å	:	$t_9 = -0.32$

[a]From Ref. 17.
[b]From Ref. 18.
[c]From Ref. 19.
[d]From Ref. 20.

localization lengths of the dimerized and undimerized polymers, because the relative disorder strength W is not identical in the two cases due to the paramterization of the hopping.

It is also interesting to compare the localization in the closely related structures of PPP, PPV, and PT. We chose to study the disorder introduced by the substitution of side chains to the phenyl and thiophene rings in the polymers, considering only the case of one side chain per ring, as in Fig. 3. A side chain, e.g., an alkyl chain, is with the same probability replacing any of the hydrogen atoms bonding to a ring. This means that there are four equivalent sites per monomer in PPP and PPV to which the side chain can bond, while PT only has two. The bonding was then simulated by changing the on-site potential by a fixed value α on one of the allowed sites, chosen randomly for every monomer. We refer to this type of disorder as the random substituent model (RSM), in contrast to the random on-site box-distribution distortion described above. Physically, the sign of α is due to the electron affinity of the side chains leading to either an enhanced or reduced electron concentration on the corresponding carbon atom. The commonly used alkoxy substituents are electron donating which corresponds to a positive α.

The inverse of λ for RSM disordered PPP is shown in Fig. 4 for different values of the disorder strength α. The
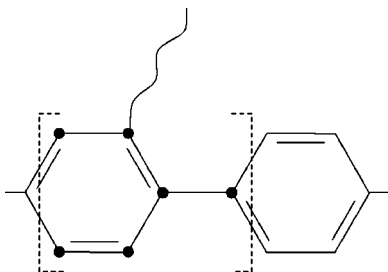

FIG. 3. The substitution of a side chain on one of four possible carbon atoms in a PPP monomer.
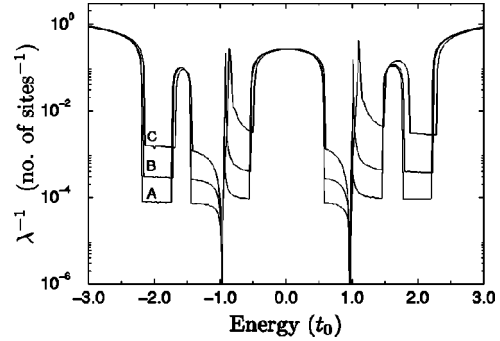

FIG. 4. The inverse of the localization length for dimerized PPP with a RSM disorder as a function of energy, plotted for different disorder strengths: $\alpha = 0.1$ (A), $\alpha = 0.2$ (B), and $\alpha = 0.5$ (C). The highest occupied molecular orbital and lowest unoccupied molecular orbital levels are -0.56 and 0.56 t_0, respectively.

energy bands of undisturbed PPP ($E \in [-2.20, -1.75]$, $[-1.45, -0.56]$, $[0.56, 1.45]$ and $[1.75, 2.20]$) are negligibly affected, but the localization length for the states within these bands is strongly reduced when α is increased.

Furthermore, the electron-hole symmetry is broken as an effect of the fixed value of the potential distortion. Changing the sign of α will result in a reflection of the curves in Fig. 4 through the zero energy point. In addition, there is a dip and a peak in the curves close to energy ± 1.0, which are not present in the random on-site box-distribution disorder results. The peaks, corresponding to a short localization length, are attributed to a small splitting of the energy bands due to the change in on-site potential of the atoms bonding to a side chain. The existence of the dips is more surprising. Actually, the states at the energies of the dips ($\pm 0.97 t_0$) are completely delocalized. This may be explained from an inspection of the corresponding wave functions of the undisturbed PPP, which are highly symmetric with zero coefficients at the atoms connecting the phenyl rings. Thus, from an energetic point of view, the rings in the RSM disordered PPP are all identical, regardless of the positioning of the substituents. This implies a complete delocalization of the wave function. One may argue that for such a wave function the transfer matrix used here fails to describe the evolution of state, since it is based on coefficients of the atoms connecting the phenyl rings, coefficients that obviously vanish. This failure is, however, restricted to a singular point and the continuity of the calculated Lyapunov exponents for energies close to this point strongly support the existence of the delocalized state. Note that it is not possible to construct a nonsingular transfer matrix for PPP describing the evolution of coefficients on any other site of the monomer.

To include the varying crystal potential of the surrounding chains, a weak random on-site box-distribution disorder on all sites was added to the RSM disorder. We shall refer to this additional disorder as noise. As shown in Fig. 5, the localization length naturally decreases with the strength of the noise, and especially the states around the dip are affected. The latter is a consequence of the small energy differences introduced between the phenyl rings, suppressing the delocalized state.

The localization length was calculated for PPP, PPV, and PT, using a RSM disorder with an additional noise of strength $W = 0.03$. In Fig. 6 the resulting localization lengths
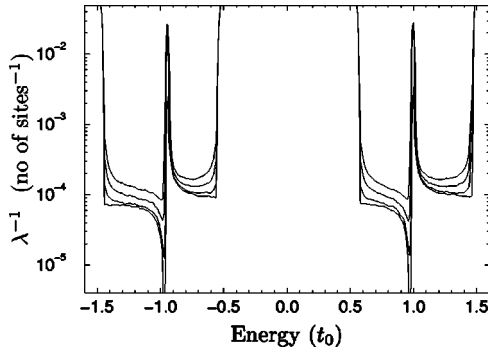
FIG. 5. The inverse of the localization length for dimerized PPP with a RSM disorder strength $\alpha = 0.1$, plus additional noise of strength W on all sites. The localization length increases with W, and the curves from the bottom and up correspond to $W=0$, $W=0.01$, $W=0.02$, and $W=0.03$.

of states close to the band gap, for both the valence and the conduction band, is presented. The chosen states were taken at a distance 0.1 t_0 from the band gap. It is clear that for this type of disorder the states in PPV will be more extended than in PPP. This is to be expected since the major disorder only affects the phenyl rings. The states in PPP and PPV are then supposed to be extended over approximately the same number of monomers. For weak RSM disorder, however, the situation is changed and the higher dimensionality of the PPP structure becomes important when the strength of the noise relative to the RSM disorder becomes substantial.

In the case of PT, the hopping to the sulfur atom is small, which implies a lower dimensionality of this polymer compared to both PPP and PPV. The correlation between localization length and dimensionality is seen clearly in Fig. 6. Moreover, the unoccupied states of PT are more extended than the occupied states. This is due to the inclusion of the sulfur atom in the wave functions of the unoccupied states, resulting in an increase of the dimensionality compared to the wave functions of the occupied states, in which the sulfur is excluded.

A large difference in localization length between occupied and unoccupied states is also present in PPP and PPV. The origin of this effect is, however, different to that of PT,
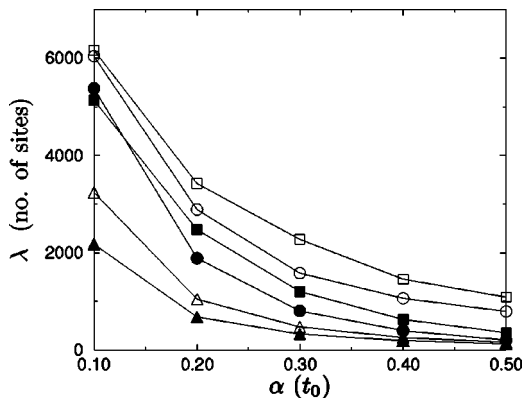

FIG. 6. The localization length for states close to the band gap of PPP (circles), PPV (squares), and PT (triangles), as a function of RSM disorder strength α. An additional noise of strength $W=0.03$ was used for all polymers. The filled symbols represent the occupied states and the hollow the unoccupied states.

and is attributed to the breaking of the electron-hole symmetry caused by the RSM and the strong influence of the delocalized singular points, as can be seen for PPP in Figs. 4 and 5. Because of the electron-hole symmetry of pristine PPP and PPV, the application of a negative RSM disorder strength α the results in Fig. 6 for occupied or the unoccupied states will be interchanged. Thus the electron affinity of the side chains determines which states that will be the most extended, the occupied or the unoccupied. The hole and electron mobilities are expected to change in the same way. This is a very interesting finding and fully explains the controversial experimental result of Hoofman *et al.*,[21] in which the intrachain mobility of electrons and holes in a dialkoxy derivative of PPV (MEH-PPV) was measured. Hoofman determined the mobility of the electrons to be roughly three times the hole mobility, in sharp contrast to bulk measurements[22] in which the hole mobility was shown to be an order of magnitude higher than the electron mobility. The alkoxy substituents are electron donating[23] which corresponds to using a positive α in our calculations. As can be seen in Fig. 6, the calculations agree very well with the findings of Hoofman, and the higher intrachain electron mobility can be understood as an effect of the particular electron affinity of the dialkoxy side chains. In the case of a bulk material, interchain interactions determine the overall mobility which may then be very different from that in the single chain. In the case of PT, no electron-hole symmetry exists, and a change of sign on α has a negligible effect on the PT localization length. In the presence of alkoxy substituents both PPP and PT are expected to have a higher electron than hole intrachain mobility, just as in PPV. This effect should be seen in experiments on PPP and PT utilizing the technique of Hoofman.

IV. CONCLUSIONS

To conclude, a general method for obtaining transfer matrices in quasi-1D systems has been developed. The simplicity of the method makes it suitable for complex systems. The restrictions on the choice of unit cell is not clear though, a matter that calls for additional studies. The method was used for some common conjugated polymers to study Anderson localization, especially the role of dimension on a molecular level was investigated. By applying two different types of disorder we showed that it is certainly meaningful to speak of different dimensionality of quasi-1D systems, and that this is an important concept for understanding Anderson localization in such systems. Due to the importance of interchain interactions for transport in polymer systems, experiments concerning isolated chains are very hard to perform. Recent techniques however have been used to determine the intrachain electron and hole mobilities in a single chain of MEH-PPV. We explain the observed higher electron mobility compared to the hole mobility as being an effect of the strong influence of some delocalized states, for which the electron-hole symmetry is broken because of the side chains.

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