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Random interchain coupling of conjugated polymers

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Abstract. Modelling the fact that the three-dimensional structure of most real conjugated polymers is not crystalline we introduce a random contribution to the perpendicular interchain hopping of the π electrons. Using a supersymmetric path integral technique the electronic density of states is calculated. It is found that the dimerization amplitude is reduced. Various technical complications with the present approach are pointed out.

1. Introduction

Since the pioneering work of Su *et al* [1] presenting a microscopic model for polyacetylene, conjugated polymers have been intensively studied from the point of view as quasi-one-dimensional electron-phonon systems. Especially in the continuum version [2] of the SSH model, physical properties such as the Peierls transition, structural effects and the dynamics of non-linear excitations like kinks and polarons have been explained within the framework of one-dimensional theories. Although it is known that these models have several shortcomings, e.g. the fact that the neglect of electronic correlations overestimates the dimerization of the lattice, these independent electron models can also give a qualitative insight, predicting the consequences of defects and disorder. However one has to keep in mind that the more complicated three-dimensional structure of real polymers includes interactions between different polymer chains as well. Recent band structure calculations of crystalline polyacetylene [3] show that, in this material, adjacent chains are coupled via overlapping hydrogen orbitals causing a non-zero interchain hopping matrix element. Assuming a perfectly ordered lattice the main features of the electronic bands can be explained by an effective tight binding model with a next nearest interchain hopping. However, in most materials, this perfect crystalline order is only locally realized. In this paper we want to study the consequences of small lattice deviations from the perfect crystallinity which give rise to a random contribution to the otherwise constant interchain hopping term. The coupling between different chains is assumed to be small compared with the intrachain next-nearest-neighbour interactions.

We employ the technique of supersymmetric functional integration following Efetov [4,5]. This method can be applied to various problems containing random potentials. For the case of *intrachain* disorder this procedure gives the exact answer; in the appendix we comment on recent results in this area.

Using the continuum version [2,8] of the SSH model the averaged Green function $G(x - x', E)$ can be expressed as a functional integral over commuting and anticommuting variables. The average over the random contribution can be performed. After

integrating out the Grassmann variables there remains the eigenvalue problem for a transfer operator. It is found that no general supersymmetric model can be formulated for more than one chain. The model Hamiltonian is divided into independent subspaces of bonding and antibonding states each having own supersymmetric properties. We will show that the application and elegance of this method is drastically restricted. Minimizing the total energy of the system (including electronic and lattice contributions) we can show that the dimerization amplitude is reduced.

2. Model and effective Hamiltonian

We start with a discrete model describing the two chains by a SSH Hamiltonian [1] and an additional interchain hopping term

$$H = H_1^{\text{SSH}} + H_2^{\text{SSH}} + H_{12} \quad (1)$$

$$H_j^{\text{SSH}} = \sum_n \left[-(t_0 - \alpha(u_{j,n+1} - u_{j,n})) (c_{j,n+1}^\dagger c_{j,n} + \text{HC}) + \frac{1}{2} K (u_{j,n+1} - u_{j,n})^2 \right] \quad (2)$$

$$H_{12} = - \sum_n t_n (c_{1,n}^\dagger c_{2,n} + \text{HC}). \quad (3)$$

As studied in [8] a constant coupling $t_n = t$ leads to a splitting of the original conduction and valence bands to bonding and antibonding states. We assume now the coupling to be site dependent and the lattice to be perfectly dimerized. In the continuum version our model then reads

$$H = \int dx \Phi^\dagger(x) h(x) \Phi(x) + \frac{\Delta^2}{\lambda} L \quad (4)$$

$$h(x) = \begin{pmatrix} -i\sigma_3 \partial_x + \sigma_1 \Delta & t(x) \\ t(x) & -i\sigma_3 \partial_x + \sigma_1 \Delta \end{pmatrix} \quad (5)$$

with four-component spinors $\Phi(x)$ describing left- and right-moving electrons on each chain, dimerization order parameter Δ , and λ the dimensionless electron-phonon coupling constant $\lambda = K/8\alpha^2$. The interchain hopping $t(x) = t + \tilde{t}(x)$ consists of a constant part t and a random part \tilde{t} with Gaussian white noise characteristics

$$\langle \tilde{t}(x) \rangle_i = 0 \quad \langle \tilde{t}(x) \tilde{t}(x') \rangle_i = \gamma \delta(x - x'). \quad (6)$$

In the discrete model, γ is the variance of the Gaussian random distribution of the interchain hopping t_n at the site n .

We use the supersymmetric method following Efetov [4,5] to obtain the averaged electronic density of states of the system. Introducing four-component commuting and anticommuting fields s, s^* and χ, χ^* the Green function of the system is written as

$$G_{\alpha\beta}(x, x', E) = \int Ds^\dagger Ds D\chi^\dagger D\chi \chi_\alpha(x) \chi_\beta^*(x') \exp \left(i \int dy L(y) \right) \quad (7)$$

with the Lagrangian

$$L = (s^\dagger(z - h)s + \chi^\dagger(z - h)\chi) \quad (8)$$

$z = E + i0$. The average over the Gaussian random contribution \bar{i} defines an effective Lagrangian \mathcal{L} via

$$\left\langle \exp \left(i \int dx L(x) \right) \right\rangle_{\bar{i}} = \exp \left(\int dx \mathcal{L}(x) \right) \tag{9}$$

and is performed using the characteristic function of Gaussian white noise

$$\left\langle \exp \left(i \int dx \bar{i}(x)g(x) \right) \right\rangle_{\bar{i}} = \exp \left(-\frac{1}{2}\gamma \int dx g^2(x) \right). \tag{10}$$

From (5) we have

$$g(x) = (\Psi_1^\dagger \Psi_3 + \Psi_2^\dagger \Psi_4 + \Psi_3^\dagger \Psi_1 + \Psi_4^\dagger \Psi_2) \quad \Psi_j = \begin{pmatrix} s_j(x) \\ \chi_j(x) \end{pmatrix}. \tag{11}$$

After an additional unitary transformation with $U = (-i1 + \sigma_1 + \sigma_2 + \sigma_3)$ in s and χ the effective Lagrangian is of the form

$$\begin{aligned} \mathcal{L} = & \Psi_1^\dagger \partial_x \Psi_2 - \Psi_2^\dagger \partial_x \Psi_1 + \Psi_3^\dagger \partial_x \Psi_4 - \Psi_4^\dagger \partial_x \Psi_3 + z(\Psi_1^\dagger \Psi_1 + \Psi_2^\dagger \Psi_2 + \Psi_3^\dagger \Psi_3 + \Psi_4^\dagger \Psi_4) \\ & - \Delta(\Psi_1^\dagger \Psi_1 - \Psi_2^\dagger \Psi_2 + \Psi_3^\dagger \Psi_3 - \Psi_4^\dagger \Psi_4) - t(\Psi_1^\dagger \Psi_3 + \Psi_2^\dagger \Psi_4 + \Psi_3^\dagger \Psi_1 + \Psi_4^\dagger \Psi_2) \\ & - \frac{1}{2}i\gamma(\Psi_1^\dagger \Psi_3 + \Psi_2^\dagger \Psi_4 + \Psi_3^\dagger \Psi_1 + \Psi_4^\dagger \Psi_2)^2. \end{aligned} \tag{12}$$

Following the approach of Fischbeck *et al* [6,7] for a single chain we define an effective Hamiltonian H corresponding to this Lagrangian via canonical conjugate fields

$$\mathcal{L} = p_1 q_1' + p_1^\dagger q_1'^\dagger + p_2 q_2' + p_2^\dagger q_2'^\dagger - H \quad q_j' = \partial_x q_j. \tag{13}$$

Corresponding to the four diagonal elements $G_{\alpha\alpha}$, $\alpha = 1, \dots, 4$ we have to define p_j and q_j in four different ways. For G_{11} we choose first

$$\begin{aligned} q_1 &= \frac{1}{\sqrt{2}}(-\Psi_1 - \Psi_3) & q_2 &= \frac{1}{\sqrt{2}}(-\Psi_1 + \Psi_3) \\ p_1 &= \frac{1}{\sqrt{2}}(-\Psi_2^\dagger - \Psi_4^\dagger) & p_2 &= \frac{1}{\sqrt{2}}(-\Psi_2^\dagger + \Psi_4^\dagger) \end{aligned} \tag{14}$$

the other combinations are given by (2) exchanging q_1 and p_1^\dagger , (3) exchanging q_2 and p_2^\dagger and (4) exchanging both q_1 and p_1^\dagger and q_2 and p_2^\dagger . These different cases lead to quite similar effective Hamiltonians, which differ just in a sign $a, b = \pm 1$ in the Δ terms

$$\begin{aligned} H_{ab} = & -z(q_1^\dagger q_1 + q_2^\dagger q_2 + p_1 p_1^\dagger + p_2 p_2^\dagger) + \Delta(a q_1^\dagger q_1 + b q_2^\dagger q_2 - a p_1 p_1^\dagger - b p_2 p_2^\dagger) \\ & + t(q_1^\dagger q_1 - q_2^\dagger q_2 + p_1 p_1^\dagger - p_2 p_2^\dagger) - \frac{1}{2}i\gamma(q_1^\dagger q_1 - q_2^\dagger q_2 + p_1 p_1^\dagger - p_2 p_2^\dagger)^2. \end{aligned} \tag{15}$$

Following the ideas of Feynman [9] the remaining functional integral in equation (7) with x playing the role of time can be performed with the help of a transfer operator technique described in detail in [3,4]. In the following we drop the ab indices and keep in mind that we have to deal with four distinct Hamiltonians. The averaged Green function $\mathcal{G}(0, E) = (\sum_{\alpha=1}^4 G_{\alpha\alpha}(x, x, E))_i$, which we need to evaluate the density of states can be expressed through the eigenstates ψ_n of H

$$H\psi_n = \varepsilon_n \psi_n \quad (16)$$

$$\mathcal{G}(0, E) = i \sum_n \int dR |\psi_n|^2 (\chi_1^* \chi_1 + \chi_2^* \chi_2) \exp(-L \varepsilon_n) \quad (17)$$

$$dR = \frac{1}{\pi^2} ds_1^* ds_1 ds_2^* ds_2 d\chi_1^* d\chi_1 d\chi_2^* d\chi_2 \quad (18)$$

including the correct normalization condition

$$\int dR |\psi_n|^2 = 1. \quad (19)$$

To calculate the Green function $\mathcal{G}(0, E)$ in the limit of an infinite chain length L we have to solve the problem $H\psi_0 = 0$ for the lowest eigenvalue $\varepsilon_0 = 0$, which gives the only contribution in (17). We are looking for a solution ψ_0 which is supersymmetric in the same way as H , i.e. it depends only on $q_j^\dagger q_j = s_j^* s_j + \chi_j^* \chi_j$, $j = 1, 2$, the lengths in the superspaces. On account of the properties of Grassmann variables ψ_0 must be a polynomial in χ_j^* , χ_j of the form

$$\begin{aligned} \psi_0 = & \Psi_0(\rho_1, \rho_2) + \partial_{\rho_1} \Psi_0(\rho_1, \rho_2) \chi_1^* \chi_1 + \partial_{\rho_2} \Psi_0(\rho_1, \rho_2) \chi_2^* \chi_2 \\ & + \partial_{\rho_1} \partial_{\rho_2} \Psi_0(\rho_1, \rho_2) \chi_1^* \chi_1 \chi_2^* \chi_2 \end{aligned} \quad (20)$$

$$\rho_1 = s_1^* s_1 \quad \rho_2 = s_2^* s_2. \quad (21)$$

Writing (16) in the variables ρ_j and replacing the fields p_j by the canonical conjugate q_j using

$$q_j^\dagger q_j = \rho_j + \chi_j^\dagger \chi_j \quad p_j p_j^\dagger = \partial_{q_j}^\dagger \partial_{q_j} = \rho_j \partial_{\rho_j}^2 + \partial_{\rho_j} + \partial_{\chi_j^*} \partial_{\chi_j} \quad j = 1, 2 \quad (22)$$

we insert equation (15) into (20) and perform the derivations in the fermionic variables χ_j^\dagger and χ_j . Finally we arrive at the following differential equation determining Ψ_0 as

$$\begin{aligned} \{ & \rho_1 [(z-t)(\partial_{\rho_1}^2 - 1) + a \Delta(\partial_{\rho_1}^2 + 1) - \frac{1}{2} i\gamma (\rho_1(\partial_{\rho_1}^2 - 1)^2 + 2(\partial_{\rho_1}^2 - 1)\partial_{\rho_1})] \\ & + \rho_2 [(z+t)(\partial_{\rho_2}^2 - 1) + b \Delta(\partial_{\rho_2}^2 + 1) - \frac{1}{2} i\gamma (\rho_2(\partial_{\rho_2}^2 - 1)^2 \\ & + 2(\partial_{\rho_2}^2 - 1)\partial_{\rho_2})] + i\gamma [\rho_1 \rho_2 (\partial_{\rho_1}^2 - 1)(\partial_{\rho_2}^2 - 1) - \partial_{\rho_1} \partial_{\rho_2}] \} \\ & \times \Psi_0(\rho_1, \rho_2) = 0 \end{aligned} \quad (23)$$

which has to be solved in the positive ρ_1, ρ_2 plane.

Using the expansion (20) for the lowest transfer function and performing the integrals over the Grassmann variables the expression for the Green function (17) is transformed into

$$\begin{aligned} \mathcal{G}(0, E) &= i \frac{\int_0^\infty d\rho_1 d\rho_2 (\Psi_0(\partial_{\rho_1} + \partial_{\rho_2})\Psi_0)}{\int_0^\infty d\rho_1 d\rho_2 (\Psi_0 \partial_{\rho_1} \partial_{\rho_2} \Psi_0 + \partial_{\rho_1} \Psi_0 \partial_{\rho_2} \Psi_0)} \\ &= i \frac{\int_0^\infty d\rho_1 |\Psi_0(\rho_1, 0)|^2}{|\Psi_0(0, 0)|^2} + i \frac{\int_0^\infty d\rho_2 |\Psi_0(0, \rho_2)|^2}{|\Psi_0(0, 0)|^2}. \end{aligned} \quad (24)$$

It is a special property of supersymmetry that we have to solve the eigenvalue problem of the effective Hamiltonian not in the complete $\{\rho_1, \rho_2\}$ plane but only at the boundary. The eigenfunction Ψ_0 is regular, which implies that all partial derivatives are finite. Therefore the differential equation (23) can be reduced to the following coupled equations

$$\begin{aligned} \{ \rho_1 [(z - t)(\partial_{\rho_1}^2 - 1) + a \Delta(\partial_{\rho_1}^2 + 1) - \frac{1}{2} i \gamma (\rho_1(\partial_{\rho_1}^2 - 1)^2 + 2(\partial_{\rho_1}^2 - 1)\partial_{\rho_1})] \} \Psi_0(\rho_1, 0) \\ = i \gamma \partial_{\rho_1} \partial_{\rho_2} \Psi_0(\rho_1, \rho_2) |_{\rho_2=0} \end{aligned} \quad (25)$$

$$\begin{aligned} \{ \rho_2 [(z + t)(\partial_{\rho_2}^2 - 1) + b \Delta(\partial_{\rho_2}^2 + 1) - \frac{1}{2} i \gamma (\rho_2(\partial_{\rho_2}^2 - 1)^2 + 2(\partial_{\rho_2}^2 - 1)\partial_{\rho_2})] \} \Psi_0(0, \rho_2) \\ = i \gamma \partial_{\rho_1} \partial_{\rho_2} \Psi_0(\rho_1, \rho_2) |_{\rho_1=0}. \end{aligned} \quad (26)$$

We cannot in general choose a solution $\Psi_0(\rho_1, \rho_2)$ with a vanishing first derivative at the boundary of the form $\partial_{\rho_1} \Psi_0(\rho_1, \rho_2)|_{\rho_1=0} = 0$. This can be seen from the boundary conditions for the original eigenvalue problem formulated in the variable $r_j = (q_j^\dagger q_j)^{1/2}$. Due to the even parity of the effective Hamiltonian the eigenfunctions for a fixed value r_2 can be written as series

$$\Psi_n(r_1, r_2) = \sum_{m=0}^{\infty} a_{nm}(r_2) r_1^{2m} \quad (27)$$

with $\Psi_n(0, r_2) = a_{n0}$, $\partial_{\rho_1} \Psi_n(\rho_1, \rho_2)|_{\rho_1=0} = 0$. The second derivative is determined by the condition that $\Psi_n(\infty, r_2)$ must be zero. Changing the variables from r_j to $\rho_j = r_j^2$ we obtain $\partial_{r_1}^2 \Psi_n(r_1, r_2)|_{r_1=0} = 2\partial_{\rho_1} \Psi_n(\rho_1, \rho_2)|_{\rho_1=0}$. Therefore the two effective equations are always coupled by a term proportional to the small quantity γ . If $\Psi_0(\rho_1, \rho_2)$ can be separated into the product $\phi_1(\rho_1) \cdot \phi_2(\rho_2)$, then equation (24) can be written as

$$\begin{aligned} \mathcal{G}(0, E) &= \sum_{a=\pm 1} \frac{\int_0^\infty d\rho_1 |\phi_1(\rho_1)|^2}{|\phi_1(0)|^2} + \sum_{b=\pm 1} \frac{\int_0^\infty d\rho_2 |\phi_2(\rho_2)|^2}{|\phi_2(0)|^2} \\ &= G_1(0, E) + G_2(0, E) \end{aligned} \quad (28)$$

with ϕ_j the solutions of the simpler equations

$$[(E \mp t)(\rho_j \partial_{\rho_j}^2 - 1) + c \Delta(\rho_j \partial_{\rho_j} + 1) - \frac{1}{2} i \gamma (\rho_j(\partial_{\rho_j}^2 - 1)^2 + 2(\partial_{\rho_j}^2 - 1)\partial_{\rho_j})] \phi_j(\rho_j) = 0 \quad (29)$$

with $c = a, b$. The decoupling approximation is justified as the additional term we have neglected does not change the asymptotic behaviour of the effective equation.

Additionally in the limit of $\gamma \rightarrow 0$ this solution is exact. In (24) the summation over the different signs a, b is equivalent to a partial summation of the diagonal elements $G_{\alpha\alpha}$ defined in equation (23c), i.e. $G_1 = G_{11} + G_{33}$, $G_2 = G_{22} + G_{44}$. A comparison with [4] shows that the differential equation (25) corresponds to the microscopic model of a single chain with only one type of on-site impurity potential responsible for forward scattering. After a Laplace transform of (25) the resulting first order equation can be solved exactly, but there is no way to perform the inverse transformation and the solution of $\phi_j(\rho)$ is given only as an integral. It can be shown [6, 7] that the integrated partial densities of states $N_j(E) = \int_0^E dE' n_j(E')$ with $n_j(E) = \pi^{-1} \text{Im} G_j(0, E)$ depend only on the value $\phi_j(0)$ which can be given exactly. With the help of these results we can write down the number of states $N(E)$ per unit length on two chains as

$$N(E) = \sum_j N_j(E) = \sum_j \frac{\gamma \sinh(\pi \epsilon_j)}{\pi^2 |I_{i\epsilon_j}(\delta)|^2} \quad \epsilon_j = \frac{E \pm t}{\gamma} \quad \delta = \frac{\Delta}{\gamma} \quad (30)$$

$I_{i\epsilon_j}(\delta)$ being the modified Bessel function of pure imaginary order.

3. Density of states and dimerization amplitude

Within our model we obtain the electronic density of states $n(E)$ for given dimerization Δ and disorder strength γ through derivation of (27) with respect to E . From the number of states $N(E)$ it can be seen that the density of states must be symmetric to the midgap energy $E = 0$. Due to the sinh terms in the numerator of $N_j(E)$ it follows that $N(+E) = -N(-E)$ and therefore $dN(+E)/dE = dN(-E)/dE$. To keep the total number of states constant a cut-off energy E_c is introduced via the relation

$$N(E_c) = N_0. \quad (31)$$

In the half-filled band case N_0 , the number of states per unit length, is equal to 2. Expanding (27) around $\Delta = 0$, $\gamma = 0$ the cut-off energy reads

$$E_c = 2\pi \left(1 + \frac{\Delta^2}{2\pi^2} - \frac{\Delta^2 \gamma^2}{2\pi^4} + \dots \right). \quad (32)$$

For arbitrary values Δ , γ the series expansion (33) is not sufficient but E_c must be computed numerically, because the total energy depends sensibly on the cut-off energy and the energetic difference between the dimerized and the normal state is very small.

The total energy of the system consists of the electronic part plus the contribution from the two perfectly dimerized lattices. We have performed numerical calculations of E_{tot}

$$E_{\text{tot}}(\Delta, \gamma) = \frac{\Delta^2}{\lambda} + N(E_c) \cdot E_c - \int_0^{E_c} dE N(E). \quad (33)$$

to study the dependence of the Peierls order parameter Δ on the disorder strength γ . First we evaluated E_c from (28) and integrated in a second step (34) numerically. We used the effective parameters typical of polyacetylene with units of the hopping

matrix element t_0 along the single chains being $\Delta(\gamma = 0) = 0.4$, which determines the dimensionless electron-phonon coupling constant λ too. The mean value of the interchain hopping t is 0.1 according to the result found in [3]. Minimizing the total energy with respect to Δ we find the actual dimerization as a function of γ . Upon increasing γ our numerical results show a continuous transition from the Peierls state with a finite dimerization amplitude to an undimerized normal state. We find a critical value $\gamma_c = 0.17$ at which the dimerization goes to zero. The Peierls order parameter Δ is shown in figure 1 as a function of the disorder strength γ .

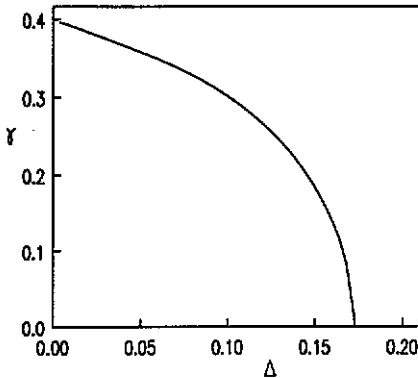


Figure 1. Dimerization order parameter Δ as function of interchain disorder strength γ .

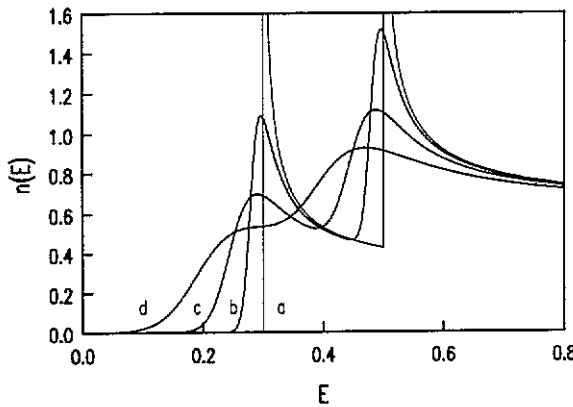


Figure 2. Density of states $n(E)$ for $E > 0$ for different values of interchain disorder strength γ : (a) $\gamma = 0.0$, (b) $\gamma = 0.004$, (c) $\gamma = 0.016$, (d) $\gamma = 0.04$

Figure 2 shows the electronic density of states corresponding to the $\Delta(\gamma)$ minimizing the total energy for different values of the disorder strength γ . Starting with $\gamma = 0$ (the case of a constant interchain hopping, i.e. in a perfectly crystalline material) the initial singularities at the band edges $E = \Delta \pm t$ become more and more smeared out with increasing γ to a double peak structure. For $\gamma = 0$ there are no states in the gap $|E| < \Delta - t$ whereas for finite γ we find a non-zero density of states.

4. Summary and conclusion

We used a supersymmetric functional integral formalism to solve the problem of two coupled chains in the presence of a random interchain hopping in the continuum description. As a result we see that this model can be mapped in the limit of small disorder strength γ to a model of two independent chains with a special kind of site disorder. In this case the energy renormalization $E \rightarrow E \pm t$ corresponds to the formation of bonding and antibonding states. The electronic density of states and the dependence of the band-order parameter Δ are calculated with the parameters of polyacetylene. Within this approximation we find a critical value of $\gamma_c = 0.17$ at which the perfectly dimerized Peierls ground state breaks down towards a metallic-like state. We have found that the order parameter Δ of this phase transition goes continuously to zero. The random interchain coupling changes the properties of the gap to a pseudogap with a small but non-zero density of states.

In contrast to the models studied in [4–7] neither the effective Hamiltonian (15) nor the effective equation (23) are invariant against supersymmetric transformations in the superspace but are divided into two subspaces of the supervectors q_1 and q_2 with separate symmetries. In these subspaces corresponding to bonding and antibonding states we can argue as usual that H depends only on the two lengths q_1 and q_2 , but no overall supersymmetry in the sense that H would be $H(q^\dagger q)$ can be reached. This is impossible because in equation (15) for the effective Hamiltonian there are terms both with $q_1^\dagger q_1 + q_2^\dagger q_2$ and $q_1^\dagger q_1 - q_2^\dagger q_2$. Even in the limit of two independent chains ($t \rightarrow 0$, $\gamma \rightarrow 0$) the effective equation separates into these two subspaces. This restricted symmetry complicates the search for eigenfunctions of the transfer operator because we have to solve a partial differential equation in two variables instead of an ordinary differential equation in the case of full supersymmetry. Although the configurational average can be performed leading to an effective Lagrangian and Hamiltonian the differential equations connected with the transfer operator technique can be solved only in the limit of small γ .

The reason for only partial supersymmetry in the case considered here lies in the fact that by the coupling of two chains the one-dimensionality necessary to obtain a full supersymmetric solution is lost. Therefore one is left with approximative methods such as small doping expansions in the effective equations, or other completely different approaches like the CPA or exact diagonalization of finite systems.

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Appendix A

In the continuum description of conducting polymers with *intrachain* disorder the Hamiltonian reads

$$H = \int dx \psi^\dagger(x) (-i\sigma_3 \partial_x + V_0(x) + (\Delta + V_1(x))\sigma_1) \psi(x) + \Delta^2/2\lambda. \quad (\text{A1})$$

with random potentials V_0 and V_1 representing bond and site impurities. In an early approach [10] to solve this problem using supersymmetric methods a mapping of equation (A1) onto a system of Schrödinger-type equations.

$$(-\partial_x^2 + (\Delta + V(x))^2 \pm dV(x)/dx)f_{\pm}(x) = E^2 f_{\pm}(x) \tag{A2}$$

with E the eigenvalue of the Dirac equation has been used (for simplicity we restrict ourselves to the case of bond impurities.) In the corresponding supersymmetric functional integral this reads for the Lagrangian

$$L = i\Phi^\dagger(\epsilon - (-\partial_x^2 + 2\Delta V + V^2 + \sigma_3 V'))\Phi \quad \epsilon = E^2 - \Delta^2. \tag{A3}$$

Now we have the first problem namely to give a meaning to $dV(x)/dx$. In general this is not possible, since e.g. a Gaussian process is not differentiable. However, mathematically it is clear that $\pm \int dx f_{\pm}(x)V'(x)f_{\pm}(x)$ can be defined via a partial integration, i.e. $\mp \int dx V(x) \partial_x(f_{\pm}(x))$. Consequently, the Lagrangian would have the form

$$L = i\Phi^\dagger(\epsilon + \partial_x^2)\Phi + iV(x)(2\Delta\Phi^\dagger\Phi - \partial_x(\Phi^\dagger\sigma_3\Phi)) + iV^2(x)\Phi^\dagger\Phi.$$

In [10] this problem is solved by an erroneous proof $\langle V'(x)V'(x') \rangle_V = 0$, which instead should give $\gamma\partial_x\partial_{x'}\delta(x-x')$.

Performing the average over $V(x)$ we then have to calculate (formally) integrals of the form $\langle \exp(\int dx \{A(x)V(x) + B(x)V^2(x)\}) \rangle_V$. First of all it is clear that this cannot be factorized into

$$\left\langle \exp\left(\int dx A(x)V(x)\right) \right\rangle_V \left\langle \exp\left(\int dx B(x)V^2(x)\right) \right\rangle_V$$

as done in [10], since obviously $V(x)$ and $V^2(x)$ are not independent. Second, since $V(x)$ is Gaussian, i.e. $\langle \dots \rangle_V = \int DV \dots \exp(-1/2\gamma \int dx V^2(x))$, one cannot give a meaning to an expression like $\langle \exp(\int dx B(x) V^2(x)) \rangle_V$ since the presence of terms quadratic in the exponential alters the normalization necessary to obtain convergent integrals. In summary, the procedure used in [10] in order to calculate an effective Lagrangian cannot be correct.

The exact solution to this problem has been given by Hayn and Fischbeck [6, 7]. If one starts from the Dirac-type equation of motion an effective Lagrangian can be derived involving only well defined averages of the form

$$\left\langle \exp\left(-i \int dx A(x)V(x)\right) \right\rangle_V = \exp\left(\int dx g(A(x))\right)$$

with g the characteristic function (here $g(y) = -\gamma y^2/2$), avoiding the problems discussed in the previous section. For the coupled chain problem discussed in the main section we have generalized their method.

So far only a Gaussian random field has been considered. If the microscopic model for the impurities is given by random positions x_j and equal strengths U , i.e. the impurity potential reads $W(x) = U \sum_j \delta(x-x_j)$, then this corresponds to a Poisson random field $V(x)$ with characteristic function $g(y) = c(\exp(-iUy) - 1)$, c impurity concentration [11]. (The use of a Gaussian random field corresponds to a quadratic

Taylor expansion of the Poisson characteristic function.) Again employing the correct supersymmetric technique the final effective equation reads

$$[-EA_- + \alpha \Delta A_+ + ic(1 - \exp(-iUA_+)]\psi_\alpha(\sigma) = 0 \quad (\text{A4})$$

with

$$A_\pm = \sigma(1 \pm \partial_\sigma^2) \quad \alpha = \pm 1. \quad (\text{A5})$$

Note that this equation is quite different than claimed in I (c). Unfortunately, it does not seem to be solvable due to the presence of derivatives of arbitrary high order.

An approximative solution in CPA to this problem has been given recently [12] which agrees quite well with numerical simulations [13].

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