PHYSICAL REVIEW B VOLUME 42, NUMBER 17 15 DECEMBER 1990-I

Impurity distribution and electronic states in doped conjugated polymers in the coherent-potential approximation

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(Received 15 May 1990)

The electronic level structure and the dimerization order parameter are studied in doped conjugated polymers when randomly distributed site-type impurities occupy different positions from those in previous investigations. Each impurity is assumed to be located at a lattice site. The number of impurities at the even-numbered sites is equal to that at the odd-numbered sites. It gives rise to both forward and backward scatterings of electrons. The generalized Takayama–Lin-Liu–Maki model is analyzed with the help of the coherent-potential approximation (CPA), using the assumption that the order parameter is uniform with one electron per site. The order parameter, the electronic level structure, and its phase diagram are obtained numerically. The characteristic CPA results obtained previously are found to be rather insensitive to the impurity positions. There are some quantitative differences. The isolated acceptor impurity band is closer to the valence band and the donor band to the conduction band at low impurity concentrations. The broadening of the density of states is reduced at high concentrations. Accordingly, the phase with an isolated impurity band becomes narrower. The phase with the vanishing energy gap also becomes narrower.

I. INTRODUCTION

In a series of studies,[1–4] we have been investigating electronic properties of conjugated polymers when they are doped by randomly distributing impurities. The Soven-Taylor coherent-potential approximation (CPA) has been applied to the generalized Takayama-Lin-Liu-Maki (TLM) model.[5] Two types of impurities have been considered: bond type giving rise to backward scattering of electrons, and site type inducing forward scattering. It has turned out[1,2] that no impurity band develops in the energy gap at low impurity concentrations when the strength of the bond component is larger than the site component. On the other hand, if the site component has a larger strength, an impurity band can be formed in the gap.[1,3] This result is different from the conventional one for semiconductors and superconductors. It is due to the one-dimensional nature of the Fermi surface, which reduces drastically the allowed phase space for scattering processes.

In the preceding paper,[3] which is referred to as I hereafter, we have pointed out the fact that, if the site-type impurities are introduced in the Su-Schrieffer-Heeger (SSH) model,[6] the local potential in the associated TLM model depends upon whether the impurities are at the $2n$th sites or at the $(2n+1)$th sites in the SSH model. To avoid the complexity, we have assumed in I that they always occupy interstitial positions between the $2n$th and $(2n+1)$th sites to give the same local potential at the two sites. This assumption has limited the impurity scatterings only to the forward processes. Using the CPA results, we have obtained a phase diagram for the electronic level structure. A phase with the isolated impurity band has been determined in the space of impurity concentration and strength. This phase occurs at low concentrations. The metallic phase with vanishing energy gap is also present in an intermediate concentration region with a rather large scattering strength.

The purpose of the present paper is to investigate how much these results depend on the assumption of interstitial doping. Therefore, we study another type of impurity distribution. We assume that impurities are evenly located at the $2n$th sites as well as at the $(2n+1)$th sites: half of the impurities are assumed to be at even-numbered sites, the other half at odd-numbered sites. We first solve a single-impurity problem. There is a localized level in the energy gap. Its energy is closer to the valence band if the impurity is an acceptor and its potential is repulsive. It is closer to the conduction band with an attractive potential. The many impurity problem is studied, under the assumption that the order parameter (size of lattice dimerization) is uniform and calculated self-consistently. The electron number is kept fixed so that half of the electronic states are filled. The electronic self-energy part is determined with the help of the CPA. We find that the electronic level structure is only quantitatively changed from that in I. In the new phase diagram, the phase with the isolated impurity band occupies a narrower region. So does the phase with the vanishing energy gap. We can, thus, conclude that the results obtained in I are qualitatively not very sensitive to the impurity positions.

In Sec. II we present the model and consider the localized state around an impurity. The many impurity problem is investigated in Sec. III, where the CPA equations are solved numerically in order to get the order parameter, level structure, and the phase diagram. The results are summarized in Sec. IV. A simplified discussion within the self-consistent Born approximation is given in the Appendix. It is found that the random distribution of the impurities, studied in the present paper, reproduces the same equations with the interstitial random distribution studied in Ref. 7.

II. SINGLE-IMPURITY PROBLEM

A site-type impurity at the mth site gives a local potential

$$H_1 = 2J \sum_s c_{ms}^\dagger c_{ms} \ , \tag{2.1}$$

to the SSH model. The operator c_{ms} annihilates an electron with spin s at the mth site and $2J$ is the strength of the impurity potential. The strength $2J$ was written J in (2.1) of I. In I, however, we assumed that the impurities are at the interstitial positions and Eq. (2.1) was replaced by (2.4). The impurity gave rise to a local potential at the two sites, each site having the strength J. In the present paper, each impurity gives rise to a local potential at only one site. The above form of H_1 would, therefore, give a J which is closer to the corresponding parameter in I. We cannot expect a direct relationship between the two J's, since the explicit form of the impurity Coulomb potential is not being taken into account. When the impurity is at an even-numbered site, $m = 2n$, the continuum limit of (2.1) is given in I to be

$$H_{\text{imp}}^{(+)} = U \sum_s \int dx \Psi_s^\dagger(x) \delta(x - x_m)(1 + \sigma_2)\Psi_s(x) \ , \tag{2.2}$$

where $\Psi_s(x)$ is a two-component field operator, $U = 2aJ$, a being the lattice constant of the undimerized system in the SSH model, $x_m = ma$, and σ_i $(i = 1, 2, 3)$ the Pauli matrices. If the impurity is at an odd-numbered site, $m = 2n + 1$, the continuum limit becomes

$$H_{\text{imp}}^{(-)} = U \sum_s \int dx \Psi_s^\dagger(x) \delta(x - x_m)(1 - \sigma_2)\Psi_s(x) \ . \tag{2.3}$$

With the single impurity, we obtain a generalized TLM model Hamiltonian

$$H = H_{\text{TLM}} + H_{\text{imp}}^{(\pm)} \ , \tag{2.4}$$

$$\begin{aligned} H_{\text{TLM}} = {} & \sum_s \int dx \Psi_s^\dagger(x) \left(-i v_F \sigma_3 \frac{\partial}{\partial x} + \Delta(x)\sigma_1 \right) \Psi_s(x) \\ & + \frac{1}{2\pi v_F \lambda} \int dx \Delta^2(x) \ , \end{aligned} \tag{2.5}$$

where v_F is the Fermi velocity, $\Delta(x)$ the order parameter, and λ the dimensionless electron-phonon coupling constant.

The order parameter is assumed not to be modified by the impurity and takes the impurity-free value $\Delta(x) = \Delta_0$. We define the temperature Green function in the impurity-free system by

$$G_s^{(0)}(k, \tau) = -\langle \mathrm{T}_\tau \Psi_s(k, \tau) \Psi_s^\dagger(k, 0) \rangle_0 \ , \tag{2.6}$$

where $\Psi_s(k, \tau) = \exp(H_0 \tau)\Psi_s(k)\exp(-H_0 \tau)$ with

$$\Psi_s(k) = \frac{1}{\sqrt{L}} \int dx e^{-ikx} \Psi_s(x) \ ,$$

L being the system size. Here, H_0 is defined by $H_0 = H_{\text{TLM}} - \mu N_e$, μ and N_e being the chemical potential and the number of electrons, respectively. Its Fourier transform with respect to τ is

$$G_s^{(0)}(k, iE_l) = (iE_l + \mu - v_F k \sigma_3 - \Delta_0 \sigma_1)^{-1} \ , \tag{2.7}$$

where $E_l = (2l + 1)\pi T$ is an odd Matsubara frequency. The Green function for the system with an impurity is

$$G_s(k, p, \tau) = -\langle \mathrm{T}_\tau \tilde{\Psi}_s(k, \tau) \tilde{\Psi}_s^\dagger(p, 0) \rangle \ , \tag{2.8}$$

where $\tilde{\Psi}_s(k, \tau) = \exp(\tilde{H}\tau)\Psi_s(k)\exp(-\tilde{H}\tau)$ with $\tilde{H} = H - \mu N_e$. Its Fourier transform satisfies the equation

$$\begin{aligned} G_s(k, p, iE_l) = {} & \delta_{k,p} G_s^{(0)}(k, iE_l) \\ & + G_s^{(0)}(k, iE_l) t(k, p, iE_l) G_s^{(0)}(p, iE_l) \ , \end{aligned} \tag{2.9}$$

where the scattering t matrix $t(k, p, iE_l)$ is given by

$$\begin{aligned} t(k, p, iE_l) = {} & \exp[i(p - k)x_m](U/L)(1 \pm \sigma_2) \\ & \times \left(1 - \frac{U}{L} \sum_{k'} G_s^{(0)}(k', iE_l)(1 \pm \sigma_2) \right)^{-1} \ . \end{aligned} \tag{2.10}$$

Using (2.7), we get

$$\frac{1}{L} \sum_{k'} G_s^{(0)}(k', iE_l) = -\frac{iE_l + \mu + \Delta_0 \sigma_1}{2 v_F [\Delta_0^2 - (iE_l + \mu)^2]^{1/2}} \ . \tag{2.11}$$

Substitution into (2.10) gives

$$\begin{aligned} t(k, p, \omega) = {} & \exp[i(p - k)x_m](U/2L)(1 \pm \sigma_2) \\ & \times [2 v_F (\Delta_0^2 - \omega^2)^{1/2} + \omega U (1 \mp \sigma_2) - \Delta_0 U (\sigma_1 \pm i \sigma_3)] / [v_F (\Delta_0^2 - \omega^2)^{1/2} + \omega U] \ , \end{aligned} \tag{2.12}$$

where iE_l is replaced by $\omega - \mu + i\delta$ by an analytic continuation with $\delta > 0$. The localized level around the impurity is determined by the singularity of $t(k,p,\omega)$, which is given by

$$(\Delta_0^2 - \omega^2)^{1/2} = -U\omega/v_F \ . \tag{2.13}$$

It has a solution

$$\omega = -U\left|\frac{\Delta_0}{U}\right|\frac{v_F}{(v_F^2+U^2)^{1/2}} \ . \tag{2.14}$$

This does not depend on whether the impurity is at an even-numbered site, (2.2), or at an odd-numbered site, (2.3). In I, the interstitially located impurity gave the localized state with the energy

$$\omega = -U\left|\frac{\Delta_0}{U}\right|\frac{4v_F^2 - U^2}{4v_F^2 + U^2} \ . \tag{2.15}$$

The absolute value of (2.14) is larger than that of (2.15) if $8v_F^2 > U^2$. This inequality would be ordinarily satisfied except for the impurities with an unreasonably large strength. The localized level is located closer to the valence band than the level obtained in I, when U is positive. It is closer to the conduction band, when U is negative.

III. COHERENT-POTENTIAL APPROXIMATION

The Hamiltonian with many impurities is written

$$H = H_{\mathrm{TLM}} + H_{\mathrm{imp}} \ , \tag{3.1}$$

$$\begin{aligned} H_{\mathrm{imp}} = {} & U\sum_{i,s}\int dx\Psi_s^\dagger(x)\delta(x-x_i^{(+)})(1+\sigma_2)\Psi_s(x) \\ & +U\sum_{i,s}\int dx\Psi_s^\dagger(x)\delta(x-x_i^{(-)})(1-\sigma_2)\Psi_s(x) \ , \end{aligned} \tag{3.2}$$

where $x_i^{(\pm)}$ indicates the position of the ith impurity. The symbol $(+)$ indicates that the impurity is at an even-numbered site, (2.2), while the symbol $(-)$ denotes the impurity at an odd-numbered site, (2.3). When the impurity concentration c is low, the possibility of two impurities occupying the neighboring sites is negligibly small. We thus suppose that each impurity independently occupies the even-numbered sites and the odd-numbered sites with an equal probability. Then, concentration of the $x_i^{(+)}$-impurities is $c/2$. The $x_i^{(-)}$-impurities have the same concentration.

We apply the coherent-potential approximation[2,3] to determine the effective-medium Green function $\bar{G}_s$ and its self-energy part Σ. They are 2×2 matrices and satisfy the equations

$$\bar{G}_s^{-1}(k,iE_l) = G_s^{(0)\ -1}(k,iE_l) - \Sigma(iE_l) \ , \tag{3.3}$$

$$\begin{aligned} & (c/2)[J(1+\sigma_2)-\Sigma]\{1-\bar{g}[J(1+\sigma_2)-\Sigma]\}^{-1} \\ & \qquad +(c/2)[J(1-\sigma_2)-\Sigma]\{1-\bar{g}[J(1-\sigma_2)-\Sigma]\}^{-1} \\ & \quad = (1-c)\Sigma(1+\bar{g}\Sigma)^{-1} \ , \end{aligned} \tag{3.4}$$

where Δ_0 in $G_s^{(0)}$ is replaced by a constant Δ, which is to be determined self-consistently, and $\bar{g} = N^{-1}\sum_k \bar{G}_s(k,iE_l)$, N being the number of sites. This is a direct generalization of (3.1) in I. We can show that Σ and $\bar{g}$ can be written as

$$\Sigma(iE_l) = \Sigma_1(iE_l) + \Sigma_2(iE_l)\sigma_1 \ , \tag{3.5}$$

$$\bar{g}(iE_l) = g_1(iE_l) + g_2(iE_l)\sigma_1 \ , \tag{3.6}$$

since the substitution into (3.4) gives

$$\begin{aligned} & c\{[(J-\Sigma_1) - g_1(J-\Sigma_1)^2 + g_1\Sigma_2^2 + J^2g_1] \\ & \qquad +[g_2(J-\Sigma_1)^2 - \Sigma_2(1+g_2\Sigma_2) - J^2g_2]\sigma_1\}/[1-2g_1(J-\Sigma_1)+2g_2\Sigma_2+(g_1^2-g_2^2)(\Sigma_1^2-\Sigma_2^2-2J\Sigma_1)] \\ & \quad = (1-c)\{[\Sigma_1 + g_1(\Sigma_1^2-\Sigma_2^2)] + [\Sigma_2 - g_2(\Sigma_1^2-\Sigma_2^2)]\sigma_1\}/[1+2(g_1\Sigma_1+g_2\Sigma_2)+(g_1^2-g_2^2)(\Sigma_1^2-\Sigma_2^2)] \ . \end{aligned} \tag{3.7}$$

There are no terms with σ_2 and σ_3. This means that the assumptions (3.5) and (3.6) do hold.

It is shown in Ref. 2 that

$$\frac{g_1(\omega)}{\omega-\Sigma_1(\omega)} = \frac{g_2(\omega)}{\Delta+\Sigma_2(\omega)} = -\frac{1}{4\pi t_0 r(\omega)}\left[\ln\left(\frac{v_F\Lambda - r(\omega)}{-v_F\Lambda - r(\omega)}\right) - \ln\left(\frac{v_F\Lambda + r(\omega)}{-v_F\Lambda + r(\omega)}\right)\right] \ , \tag{3.8}$$

where

$$r(\omega) = [(\omega-\Sigma_1)^2 - (\Delta+\Sigma_2)^2]^{1/2} \ . \tag{3.9}$$

Here, the quantity $\Lambda = a^{-1}$ is the cutoff for the k integral and the ln means the principal value of logarithm. The square root is so defined that $\mathrm{Im}\,r(\omega) > 0$ at the real axis. We take a finite Λ to keep the total number of states constant during numerical procedures.

Introducing the spectral function by

$$\tau(x) = -\frac{1}{\pi}\mathrm{Im}g_2(x) , \tag{3.10}$$

we rewrite the self-consistency equation[2] for Δ

$$4NT\sum_l g_2(iE_l) + L\frac{\Delta}{\pi\lambda v_F} = 0 , \tag{3.11}$$

to find

$$\Delta = -4\pi\lambda t_0 \int_{-\infty}^{\infty} dx f(x-\mu)\tau(x) , \tag{3.12}$$

where $f(x) = 1/[\exp(x/T)+1]$. At T=0, Eq. (3.12) becomes

$$\Delta = -4\pi\lambda t_0 \int_{-\infty}^{\mu} dx\, \tau(x) . \tag{3.13}$$

Equations (3.7), (3.8), (3.10), and (3.13) are to be solved numerically, using an iteration method as in the previous studies.

We use the parameters t_0=2.5 eV, $v_F\Lambda = 2t_0$, and λ=0.183. The order parameter of the impurity-free system is $\Delta_0 = 2v_F\Lambda\exp(-1/2\lambda) = 0.65$ eV. The value of J is varied within $|J| \lesssim t_0$. Although Eq. (3.7) may not be valid for high concentrations, we change the concentration in the range $0 \le c \le 0.5$ in order to see how different the results are from the previous results in I. We can choose a positive value for Δ without loss of generality, since the discussions of the Appendix (1) in I still hold with (3.7) of the present paper.

We take 381 points in the mesh of ω space, that is, 50 points for each sign of $\omega - cJ$ in $0.9v_F\Lambda < |\omega - cJ| \le 1.2v_F\Lambda$, 40 points for each sign of $\omega - cJ$ in $1.5\Delta < |\omega - cJ| \le 0.9v_F\Lambda$, and 201 points for $|\omega - cJ| \le 1.5\Delta$. In each energy range, they are distributed with equidistance.

First, we take an arbitrary starting value for Δ to get g_1 and g_2 by (3.8) with assumptions $\Sigma_1 = \Sigma_2 = 0$. Equation (3.7) is solved to get new Σ_1 and Σ_2, which give new g_1 and g_2 with the help of (3.8). The spectral function $\tau(x)$ is calculated by (3.10). A new Δ is obtained by (3.13). This process is iterated until the new Δ does not differ from the next new one by more than 10^{-2} percent. In each stage of the process, it is checked that the total number of states does not change more than 10^{-2} percent.

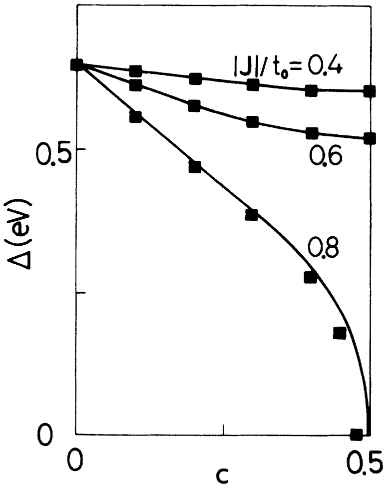

FIG. 1. The concentration dependence of the order parameter Δ for three values of $|J|/t_0$. The solid lines indicate the present results. The squares are the previous results in I. The data do not depend on the sign of J.

In Fig. 1 the concentration dependence of the order parameter Δ is presented for three values of $|J|/t_0$. The solid curves are the present results, while the squares are the previous results in I. They do not depend on the sign of J. This is the consequence of the symmetry property between the alternative signs of J as discussed in the Appendix (2) of I. The discussion still holds with (3.7) of the present paper. For $|J|/t_0 \lesssim 0.6$, the two sets of data well agree each other. The order parameter decreases linearly for a small c. The negative coefficient of the linear term can be determined by the self-consistent Born approximation, which is to be discussed in the Appendix. For $|J|/t_0 \sim 0.8$, the order parameter Δ is larger than that in I. It vanishes at $c \sim 0.5$. This critical concentration is slightly larger than that of I.

The electronic density of states per site is calculated by the formula

$$\rho(x) = -\frac{1}{\pi}\mathrm{Tr}[\mathrm{Im}\bar{g}(x)] = -\frac{2}{\pi}\mathrm{Im}g_1(x) . \tag{3.14}$$

In Fig. 2 we show the positions of the top of the valence band and the bottom of the conduction band by solid and dashed lines, respectively, for J/t_0=0.8. Thick and thin

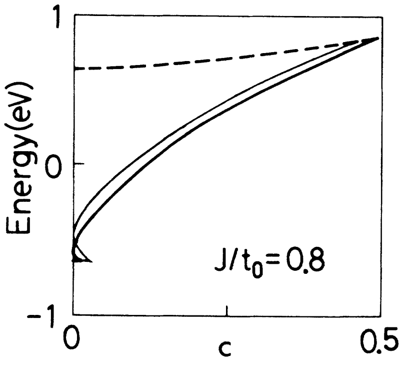

FIG. 2. The positions of the top of the valence band and the bottom of the conduction band for J/t_0=0.8. The former are indicated by solid lines and the latter by the dashed line. The thick solid line denotes the present result and the thin line the previous result in I. The structures just above the valence band at low concentrations are associated with the localized impurity band.

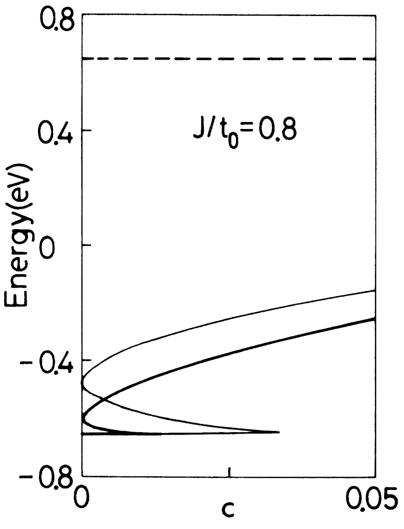

FIG. 3. The detailed drawing of Fig. 2 at low concentrations.

lines are the present and previous results, respectively. Figure 3 is the detailed drawing of the low concentration region. The structures at $c < 0.03$ are associated with the formation of the isolated impurity band just above the valence band. In the preceding section, the localized level at the single impurity is found to be energetically closer to the valence band than that in I. Accordingly, the impurity band is closer to the valence band, in the present model, and it is connected to the valence band at a lower concentration. At higher concentrations, the density of states is less broadened and the gap is wider than in I. At $c \simeq 0.5$, the energy gap vanishes. The critical concentration is slightly larger than in I. There is practically no region for the gapless dimerization, since the energy gap vanishes almost at the same time with Δ. The vanishing of the energy gap means that the main part of the valence band comes into contact with that of the conduction band.

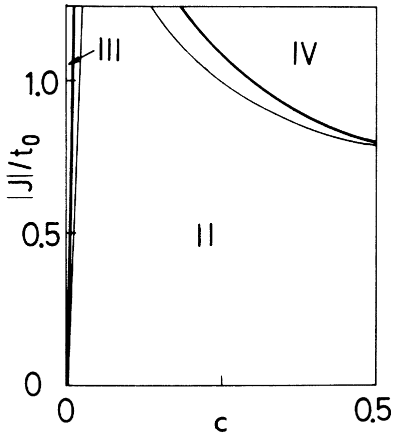

FIG. 4. Phase diagram of the electronic level structure. The thick lines indicate the phase boundaries of the present model and the thin lines are obtained in I. In phase III, there is an isolated impurity band in the energy gap. It is connected to the valence band in phase II. The energy gap vanishes in phase IV.

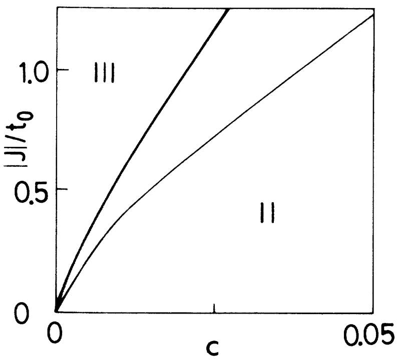

FIG. 5. The detailed drawing of Fig. 4 at the concentrations $0 \leq c \leq 0.05$.

In Fig. 4 we present the phase diagram of the electronic structure. Thick and thin lines are the phase boundaries of the present model and that in I, respectively. Figure 5 is the detailed drawing at low concentrations. The notations are the same as in Ref. 2. In phase III an isolated impurity band exists. It becomes narrower in the present model. This is already seen in Fig. 3. In phase IV the energy gap vanishes. It also becomes narrower. The remaining region is denoted by II. In this region, the impurity band is connected to the valence band at low concentrations. At higher concentrations, the impurity band merges into the valence band, forming a single broad peak.

IV. CONCLUSIONS AND DISCUSSION

We have found that the major characteristics of the electronic level structure are not so sensitive to the model of the site-type impurities. The backward scattering of electrons is taken into account with the help of the terms with σ_2 in (2.2) and (2.3). They do not qualitatively change the level structures and order parameter of the site-type impurity system with forward scatterings only.[3] Quantitatively, however, there are some differences. At low concentrations, the phase with the isolated impurity band becomes narrower. At higher concentrations, the energy gap is larger than that in I. At $c \simeq 0.5$, it vanishes when the impurity potential is strong enough. This critical concentration is slightly larger. On the other hand, the correction to the order parameter is small. For weak impurity strengths, the order parameter agrees well with that in I. At low concentrations, the concentration dependence is well explained by the self-consistent Born approximation (SCBA).[4] When the impurity strength is larger, the order parameter becomes a little larger than that in I. We can thus conclude that the characteristic CPA results obtained in I are well representing the level structures and the phase diagrams of conjugated polymers doped with the site-type impurities regardless of the detailed nature of the impurities. All the discussions are on the basis of the CPA and a uniform order parameter. It should be interesting to study the system beyond this approximation and assumption.

A few remarks on other methods seem to be in order. Baeriswyl[8] pointed out that the TLM equations with site impurities at even sites are equivalent to the model of Frisch and Lloyd[9] for a particle in a one-dimensional space in which impurities are randomly distributed with δ-function potentials. They obtained the integrated density of states by calculating the number of zeros of a wave function with given energy. The TLM equations, however, give a Frisch-Lloyd impurity strength which is proportional to the energy. Nevertheless, Baeriswyl[8] determined the density of states using the constant order parameter of the impurity-free system although it is not obvious that the method of zero counting will apply in this case. He obtained an impurity band at low concentrations which broadens with increasing concentration and finally connects to the valence band. His general trend is in agreement with our results except for the fact that he obtained additional peaks which, he claimed, come from configurations where two or more impurities are close to each other. Obviously, our single-site version of the CPA does not reproduce them.

Xu and Trullinger[10] used a supersymmetric technique, assuming a Gaussian distribution of disorder which corresponds to the Born approximation.[11] Recently, Xu and Taylor[12] pointed out that this technique can be used with a Poisson distribution to get a Frisch-Lloyd equation. This equation shows, however, that the effective site-type impurity strength is again proportional to the energy. It would be interesting to find relations with the conclusions of Wegner[13] who proved the nonexistence of zeros and singularities in the density of states for a wide class of disordered systems, with the exception of certain cases. It appears that the TLM model is an example of such exceptions with the Gaussian distribution.[14] But, it is unclear if this is true for the Poisson case.

ACKNOWLEDGMENTS

The authors acknowledge the discussions with Professor Y. Ono, Dr. A. Terai, Dr. K. Iwano, Dr. T. Ohtsuki, and Dr. K. Yonemitsu. This work has been supported by Deutsche Forschungsgemeinschaft through Sonderforschunsbereich 213 (Topomak, Bayreuth). Numerical calculations have been performed on HITAC M-680 and S-820 in the computer center of Institute for Molecular Science, Okazaki National Research Institutes, Japan.

APPENDIX: SELF-CONSISTENT BORN APPROXIMATION

It was shown in the previous studies[7] that with the method of the SCBA the problem of doped conjugated polymers with uniform dimerization can be mapped onto the equations of a superconductor with magnetic impurities. Site-type impurities have been assumed at the interstitial sites giving rise to forward scattering of electrons only. It would be of some interest to see if the impurity distribution, as discussed in this paper, would modify this mapping.

In the SCBA, the self-energy part $\Sigma(iE_l)$ is given by

$$\begin{aligned}\Sigma(iE_l) = {} & (c/2)[J(1+\sigma_2)+J(1-\sigma_2)] \\ & +(c/2)[J(1+\sigma_2)\bar{g}(iE_l)J(1+\sigma_2) \\ & +J(1-\sigma_2)\bar{g}(iE_l)J(1-\sigma_2)]\ . \qquad \text{(A1)}\end{aligned}$$

Substitution of (3.5) and (3.6) gives

$$\Sigma_1(iE_l) = cJ + 2cJ^2 g_1(iE_l)\ , \qquad \text{(A2)}$$

and

$$\Sigma_2(iE_l) = 0\ . \qquad \text{(A3)}$$

The first term of (A2) gives a shift of the energy and is therefore neglected.

Combining (3.3), (3.5), and (3.6), we get

$$\begin{aligned} g_1(\omega) &= -\frac{\omega-\Sigma_1}{2t_0[\Delta^2-(\omega-\Sigma_1)^2]^{1/2}} \\ &= -\frac{u}{2t_0\sqrt{1-u^2}}\ , \qquad \text{(A4)}\end{aligned}$$

and

$$\begin{aligned} g_2(\omega) &= -\frac{\Delta}{2t_0[\Delta^2-(\omega-\Sigma_1)^2]^{1/2}} \\ &= -\frac{1}{2t_0\sqrt{1-u^2}}\ , \qquad \text{(A5)}\end{aligned}$$

where the relation $v_F = 2at_0$ in the SSH model is used. Here, an analytic continuation to the real axis, $iE_l + \mu \rightarrow \omega + i\delta$, is performed and the square root is so defined that $\mathrm{Re}\sqrt{\ } > 0$. The complex variable u is introduced by

$$u = \frac{\omega - \Sigma_1}{\Delta}\ . \qquad \text{(A6)}$$

Equation (A6) is rewritten, with the help of (A2), (A3), (A4), and (A5),

$$\frac{\omega}{\Delta} = u\left(1 - \frac{\zeta}{\sqrt{1-u^2}}\right)\ , \qquad \text{(A7)}$$

where $\zeta = cJ^2/\Delta t_0$. These are the same equations as those in Ref. 7. The self-consistency equation for Δ, (3.11), is also the same. We, thus, find that the distribution of the site-type impurities, as discussed in this paper does not change the SCBA equations.

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