Interchain coupling model for quasi-one-dimensional π-conjugated organic ferromagnets

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Two neighboring π-conjugated organic-polymer ferromagnetic chains are described individually by a Hamiltonian, which is the Su-Schrieffer-Heeger Hamiltonian added by the Hubbard electron-electron repulsion. In consideration of the topological structure of the system, the interchain coupling is taken into account as an interchain electron-transfer term, which is different with respect to different sites in chains. The splitting of energy levels with respect to different chains, the ferromagnetic order, and the dimerization are studied in detail. It is shown that in the high-spin ground state of the system, different configurations with interchain coupling will result in transfer of spin density between the main chain and side radical, and appropriate coupling strength stabilizes the high-spin ground state. However, as the coupling reaches a critical value, the energy gap disappears and the high-spin state does not exist. It is also found that the dimerization along the main chain varies with the interchain coupling. [S0163-1829(97)11016-5]

I. INTRODUCTION

Since several quasi-one-dimensional organic ferromagnets such as DTDA (N,N'-dioxy-1,3,5,7-tetramethyl-2,b-diazaadamantane) (Ref. 1) and p-NPNN (p-nitrophenyl nitronyl nitroxide) (Ref. 2) have been successfully synthesized, a new class of ferromagnetic materials based on molecular rather than metallic lattices has attracted considerable attention.[3–8] However, little is known about the mechanism of ferromagnetism in these organic materials.

Ovchinnikov and Spector[9] proposed a simplified structure of quasi-one-dimensional organic polymer ferromagnets schematically shown in Fig. 1. The main chain consists of carbon atoms that each have a π electron and R is a kind of side radical containing an unpaired electron. They treated the π electrons along the main carbon chain as an antiferromagnetic spin chain, and assumed that there exists an antiferromagnetic correlation between the π-electron spin and the residual spin of side radical. Recently, Fang, Liu, and Yao[10,11] proposed a theoretical model to describe this kind of quasi-one-dimensional organic ferromagnet. They considered the itineracy of π electrons, the Hubbard electron-electron correlation, and the antiferromagnetic spin correlation between the π electrons and unpaired electrons at side radicals. Within the mean-field theory, they calculated the energy levels that split off with respect to different spins. In the ferromagnetic ground state, there exists a spin-density wave with alternation of the sign and the amplitude of the spin density along the main chain. In fact, the unpaired electrons at side radicals is not totally localized. They can hop between the main chain and the side radicals. Fang, Liu, and Yao[12] also discussed this situation and obtained a ferromagnetic ground state with high spin. However, in their works, the system was treated as an isolated chain. Since there is no purely one-dimensional system, in certain situations, interchain interaction can have a significant effect as will be demonstrated in this paper. In this paper we propose an interchain coupling model and it is shown that due to interchain coupling, the degeneracy of energy levels with respect to different chains is lifted. The distribution of spin density is influenced dramatically and the dimerization is different from the one-dimensional system.

In our model, the interchain coupling is considered to be an interchain electron transfer between the corresponding sites on nearest chains. Due to the topological structure of the system, the interchain couplings are different with respect to different sites in the chains. This is similar to the situations in typical organic polymers with chainlike structure, such as polyacetylene[13–15] and polyacene,[16] in which the interchain interaction is interchain hopping of electrons, but phonons are strictly one dimensional. In Sec. II, we give the model Hamiltonian describing the hopping of the π electrons on the main chain and the unpaired electrons at the side radicals, the Hubbard electron-electron repulsion, and the interchain coupling. The numerical procedures employed in our work are also given in Sec. II. The results and discussions are given in Sec. III.
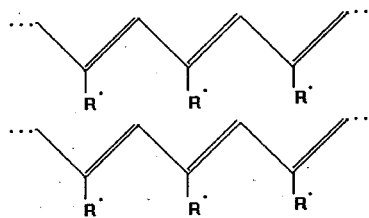

FIG. 1. Two neighboring chains of a quasi-one-dimensional organic ferromagnet.
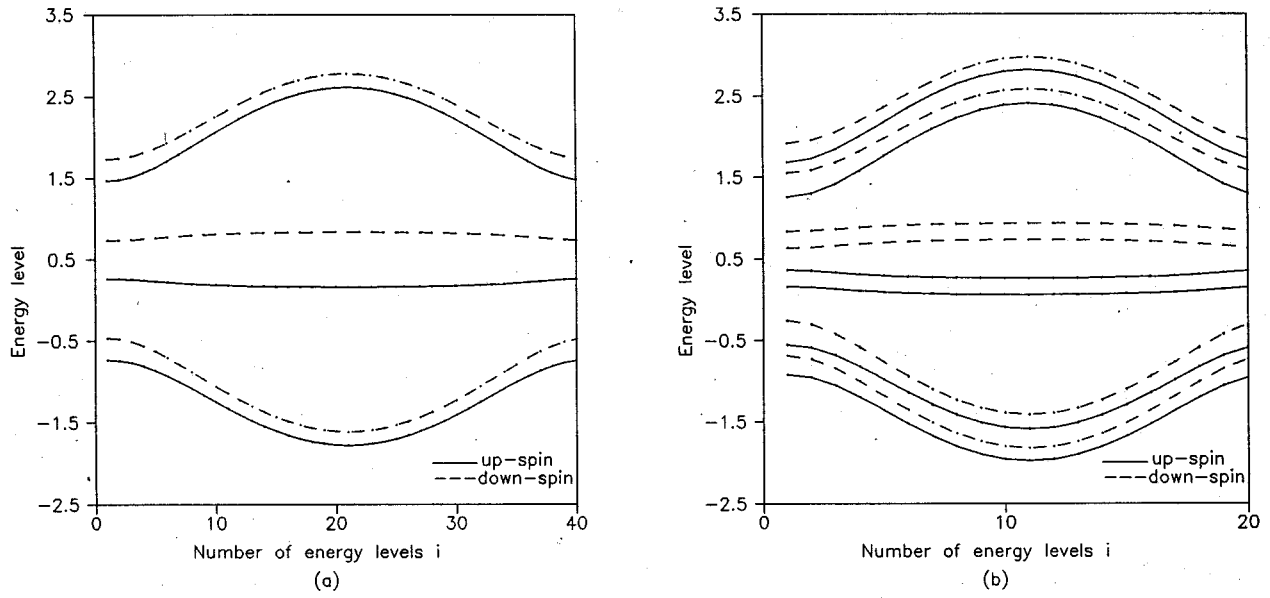
FIG. 2. The energy spectra (a) without interchain coupling, (b) with the interchain coupling $t_2 = 0.1$, $t_3 = 0.3$, $t_4 = 0.1$; i indicates the number of the energy levels.

II. THE MODEL HAMILTONIAN AND NUMERICAL PROCEDURE

We consider two neighboring coupled chains shown in Fig 1. Based on the discussion in Sec. I, the Hamiltonian employed in our study can be written as

$$H = H_0 + H', \tag{1}$$

where H_0 is the Hamiltonian of two isolated chains and H' describes the interchain coupling. We can write H_0 explicitly as follows:

$$H_0 = H_1 + H_2, \tag{2}$$

$$H_1 = -\sum_{jl\sigma} [t_0 + \gamma(u_{jl} - u_{jl+1})](c^{\dagger}_{j1l\sigma} c_{j1l+1\sigma} + \text{H.c.})$$

$$- \sum_{jl\sigma} (T_1 c^{\dagger}_{j1l\sigma} c_{j2l\sigma} \delta_l + \text{H.c.}) + \frac{\kappa}{2} \sum_{jl} (u_{jl} - u_{jl+1})^2, \tag{3}$$

$$H_2 = U \sum_{jl} (n_{j1l\alpha} n_{j1l\beta} + n_{j2l\alpha} n_{j2l\beta} \delta_l). \tag{4}$$
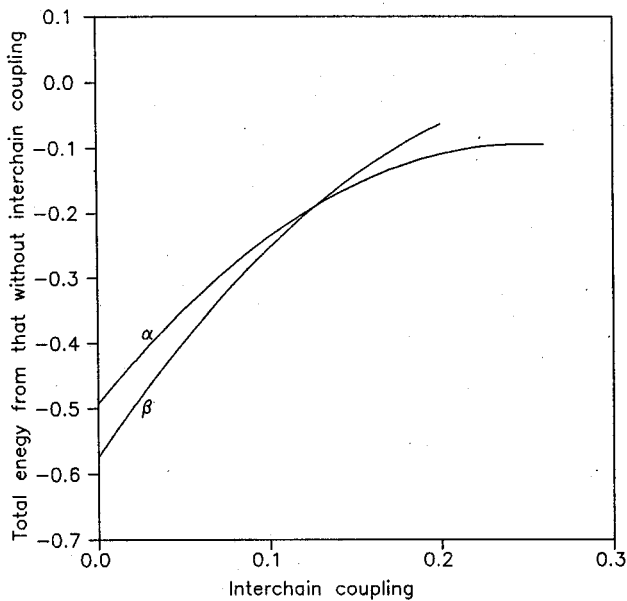

FIG. 3. The total energy of the system from that without interchain coupling vs the interchain coupling t_2. Curve α is for $t_3 = 0.3$, $t_4 = 0.1$; curve β is for $t_3 = 0.3$, $t_4 = 0.3$.
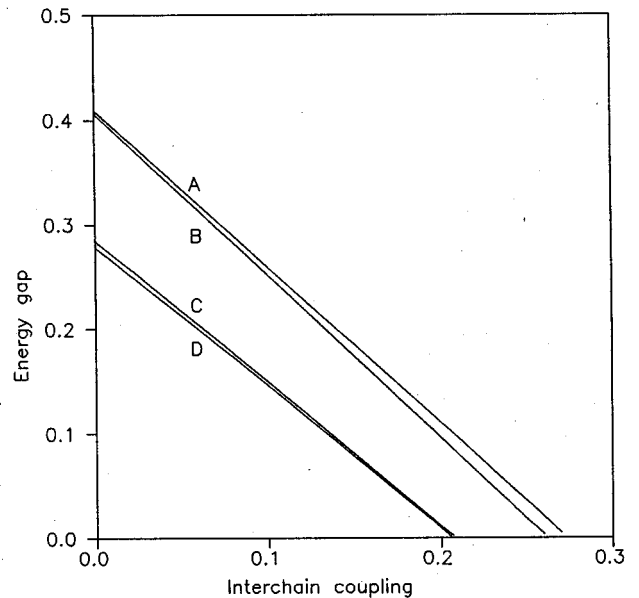
FIG. 4. The energy gap vs the interchain coupling t_2. Curve A is for $t_3 = 0.1$, $t_4 = 0.1$; curve B is for $t_3 = 0.3$, $t_4 = 0.1$; curve C is for $t_3 = 0.1$, $t_4 = 0.3$; curve D is for $t_3 = 0.3$, $t_4 = 0.3$.
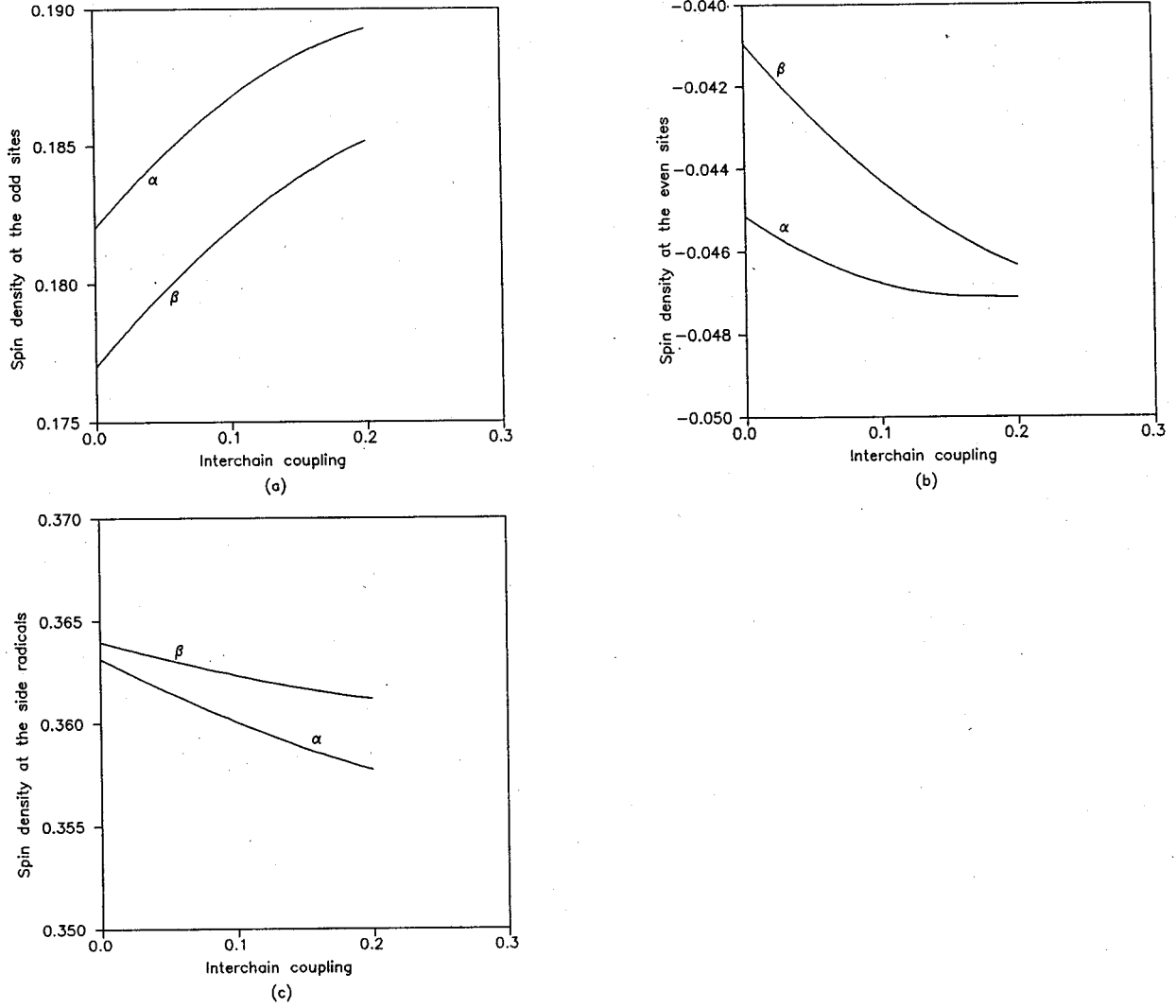
FIG. 5. The spin density at different sites vs the interchain coupling t_2; (a) at the odd sites on each main chain; (b) at the even sites on each main chain; (c) at the side radicals. Curve α is for $t_3 = 0.3$, $t_4 = 0.1$; curve β is for $t_3 = 0.3$, $t_4 = 0.3$.

The first term H_1 describes the intrachain hoppings of the π electrons on each main chain and the unpaired electrons at the side radicals, the electron-phonon interaction, and the distortion of the lattice, where $c^\dagger_{jil\sigma}$ ($c_{jil\sigma}$) denotes the creation (annihilation) operator of a π electron ($i = 1$) along each main chain or an unpaired electron ($i = 2$) at a side radical with spin σ on the lth site in the jth chain, t_0 is the hopping integral of the π electron along each main chain when there is no dimerization, T_1 is the hopping integral between a π electron on the main chain and an unpaired electron at the side radical, γ is the electron-phonon coupling constant, u_{jl} is the displacement of the lth site on the jth main chain, and κ is the elastic constant of the lattice. We assume that the side radicals connect with the even carbon atoms; then

$$\delta_l = 1 \quad (l \text{ even}),$$

$$\delta_l = 0 \quad (l \text{ odd}). \tag{5}$$

The second term H_2 describes the Hubbard electron-electron repulsions of π electrons (the first term in H_2) and

unpaired electrons at the side radicals (the second term in H_2). $n_{jil\sigma} = c^\dagger_{jil\sigma} c_{jil\sigma}$ ($\sigma = \alpha, \beta$) where α and β denote up-spin and down-spin, respectively.

Considering the topological structure of the system, we assume the interchain coupling in the following form:

$$H' = -\sum_{l\sigma} [T_2(1 - \delta_l) + T_3\delta_l](c^\dagger_{11l\sigma} c_{21l\sigma} + \text{H.c.})$$

$$-T_4 \sum_{l\sigma} (c^\dagger_{12l\sigma} c_{22l\sigma}\delta_l + \text{H.c.}), \tag{6}$$

where T_2 (T_3) are interchain electron transfers from the odd site (even site) in the first chain to the corresponding odd site (even site), T_4 is the interchain hopping integral from the side radical in the first chain to the corresponding side radical in the second one.

It is convenient to cast all quantities into dimensionless forms as

$$h = \frac{H}{t_0}, \quad u = \frac{U}{t_0}, \quad t_i = \frac{T_i}{t_0} \quad (i=1,2,3,4),$$

$$\lambda = \frac{2\gamma^2}{t_0\pi\kappa}, \quad y_{jl} = (-1)^l(u_{jl} - u_{jl+1})\gamma/t_0. \tag{7}$$

So the Hamiltonian h becomes

$$h = h_e + h', \tag{8}$$

$$h_3 = -\sum_{jl\sigma} [1+(-1)^l y_{jl}](c^{\dagger}_{j1l\sigma}c_{j1l+1\sigma} + \text{H.c.})$$

$$-\sum_{jl\sigma} (t_l c^{\dagger}_{j1l\sigma}c_{j2l\sigma}\delta_l + \text{H.c.})$$

$$+u\sum_{jl} (n_{j1l\alpha}n_{j1l\beta} + n_{j2l\alpha}n_{j2l\beta}\delta_l)$$

$$-\sum_{l\sigma} (t_4 c^{\dagger}_{12l\sigma}c_{22l\sigma}\delta_l + \text{H.c.})$$

$$-\sum_{l\sigma} [t_2(1-\delta_l) + t_3\delta_l](c^{\dagger}_{11l\sigma}c_{21l\sigma} + \text{H.c.}), \tag{9}$$

$$h' = \frac{1}{\pi\lambda}\sum_{jl} y_{jl}^2, \tag{10}$$

where h_e is the electronic part of the Hamiltonian, and h' describes the elastic energy of the lattice.

Since we use the tight-binding approximation in the Hamiltonian [Eq. (1)], the wave function of the system can be expanded in site basis functions in the Wannier representation:[17]

$$\Psi_{\mu} = \sum_{jil\sigma} Z^{\sigma}_{\mu jil} c^{\dagger}_{jil\sigma}|0\rangle, \tag{11}$$

where $|0\rangle$ is the true electron vacuum state, Ψ_{μ} denotes the μth eigenvector of the Hamiltonian, $Z^{\sigma}_{\mu jil}$ is the expansion coefficient. In fact, the tight-binding approximation should be confirmed by the feature of the wave function appearing as a result of numerical calculations. We assume that the π electrons along the main chain and the unpaired electrons at the side radicals are relatively localized. Hence, we use the tight-binding approximation for the quasi-one-dimensional organic ferromagnet as that in Su-Schrieffer-Heeger model[18] for polyacetylene with similar chainlike structure.

We will numerically solve the Schrödinger equation of the system:

$$h_e\Psi_{\mu} = \varepsilon_{\mu}\Psi_{\mu}. \tag{12a}$$

Here, ε_{μ} is the μth eigenvalue of Eq. (12a). From Eqs. (11) and (12a), we can write the eigenvalue equation explicitly:

$$\langle 0|c_{j'i'l'\sigma'}h_e\sum_{jil\sigma} Z^{\sigma}_{\mu jil} c^{\dagger}_{jil\sigma}|0\rangle$$

$$= \varepsilon^{\sigma}_{\mu}\langle 0|c_{j'i'l'\sigma'}\sum_{jil\sigma} Z^{\sigma}_{\mu jil} c^{\dagger}_{jil\sigma}|0\rangle, \tag{12b}$$

namely,

$$-[1+(-1)^l y_{jl}]Z^{\sigma}_{\mu11l+1} - [1+(-1)^{l-1}y_{jl-1}]Z^{\sigma}_{\mu11l-1}$$

$$-t_1\delta_l Z^{\sigma}_{\mu12l} + u\left(\sum_{\substack{\mu'\\(\text{occ})}} Z^{\bar{\sigma}}_{\mu'11l}Z^{\bar{\sigma}*}_{\mu'11l}\right)Z^{\sigma}_{\mu11l} - [t_2(1-\delta_l)$$

$$+t_3\delta_l]Z^{\sigma}_{\mu21l} = \varepsilon^{\sigma}_{\mu}Z^{\sigma}_{\mu11l}, \tag{13}$$

$$u\left(\sum_{\substack{\mu'\\(\text{occ})}} Z^{\bar{\sigma}*}_{\mu'12l}\right)Z^{\sigma}_{\mu12l}\delta_l - t_1Z^{\sigma}_{\mu11l}\delta_l - t_4Z^{\sigma}_{\mu22l}\delta_l = \varepsilon^{\sigma}_{\mu}Z^{\sigma}_{\mu12l}, \tag{14}$$

$$-[1+(-1)^l y_{jl}]Z^{\sigma}_{\mu21l+1} - [1+(-1)^{l-1}y_{jl-1}]Z^{\sigma}_{\mu21l-1}$$

$$-t_1\delta_l Z^{\sigma}_{\mu22l} + u\left(\sum_{\substack{\mu'\\(\text{occ})}} Z^{\bar{\sigma}}_{\mu'22l}Z^{\bar{\sigma}*}_{\mu'21l}\right)Z^{\sigma}_{\mu21l} - [t_2(1-\delta_l)$$

$$+t_3\delta_l]Z^{\sigma}_{\mu11l} = \epsilon^{\sigma}_{\mu}Z^{\sigma}_{\mu21l}, \tag{15}$$

$$u\left(\sum_{\substack{\mu'\\(\text{occ})}} Z^{\bar{\sigma}}_{\mu'22l}Z^{\bar{\sigma}*}_{\mu'22l}\right)Z^{\sigma}_{\mu22l}\delta_l - t_1Z^{\sigma}_{\mu21l}\delta_l - t_4Z^{\sigma}_{\mu12l}\delta_l$$

$$= \epsilon^{\sigma}_{\mu}Z^{\sigma}_{\mu22l}. \tag{16}$$

Here, $\bar{\sigma} = \alpha\delta_{\beta\sigma} + \beta\delta_{\alpha\sigma}$, and we have used the mean-field approximation to divide $n_{jil\sigma}$ as follows:

$$n_{jil\sigma} = \langle n_{jil\sigma}\rangle + \Delta n_{jil\sigma}, \tag{17}$$

where $\langle\ \rangle = \langle G|\cdots|G\rangle$ is the average with respect to the ground state $|G\rangle$, $\Delta n_{jil\sigma}$ is fluctuation from the average value.

The total energy of the system with the Hamiltonian [Eq. (8)] is

$$E(\{y_{jl}\}) = -\sum_{jl\sigma} [1+(-1)^l y_{jl}]\sum_{\substack{\mu\\(\text{occ})}} (Z^{\sigma*}_{\mu j1l+1}Z^{\sigma}_{\mu j1l}$$

$$+Z^{\sigma*}_{\mu j1l}Z^{\sigma}_{\mu j1l+1}) + \frac{1}{\pi\lambda}\sum_{jl} y_{jl}^2$$

$$-t_1\sum_{jl\sigma}\sum_{\substack{\mu\\(\text{occ})}} (Z^{\sigma*}_{\mu j1l}Z^{\sigma}_{\mu j2l} + Z^{\sigma*}_{\mu j2l}Z^{\sigma}_{\mu j1l})\delta_l$$

$$-\sum_{l\sigma} t_4\sum_{\substack{\mu\\(\text{occ})}} (Z^{\sigma*}_{\mu12l}Z^{\sigma}_{\mu22l} + Z^{\sigma*}_{\mu22l}Z^{\sigma}_{\mu12l}) - \sum_{l\sigma} [t_2(1$$

$$-\delta_l) + t_3\delta_l]\sum_{\substack{\mu\\(\text{occ})}} (Z^{\sigma*}_{\mu11l}Z^{\sigma}_{\mu21l} + Z^{\sigma*}_{\mu21l}Z^{\sigma}_{\mu11l})$$

$$+u\sum_{jl}\left(\sum_{\substack{\mu\mu'\\(\text{occ})}} |Z^{\alpha}_{\mu j1l}|^2|Z^{\beta}_{\mu'j1l}|^2\right.$$

$$\left. +\sum_{\substack{\mu\mu'\\(\text{occ})}} |Z^{\alpha}_{\mu j2l}|^2|Z^{\beta}_{\mu'j2l}|^2\delta_l\right). \tag{18}$$
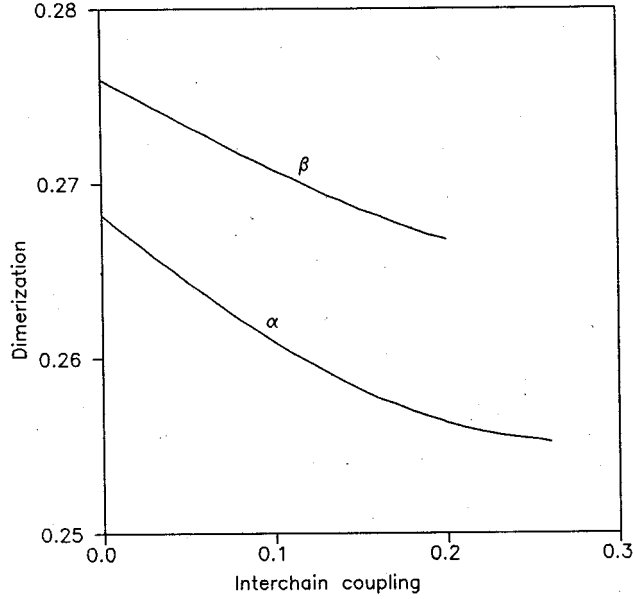
FIG. 6. The dimerization vs the interchain coupling t_2. Curve α is for $t_3 = 0.3$, $t_4 = 0.1$; curve β is for $t_3 = 0.3$, $t_4 = 0.3$.

The dimerization y_{jl} can be obtained by minimizing the total energy of the system with respect to y_{jl}:

$$
y_{jl} = \pi\lambda(-1)' \left[\sum_{\substack{\mu\sigma \\ (\text{occ})}} Z^\sigma_{\mu j 1 l} Z^\sigma_{\mu j 1 l+1} \right.
$$

$$
\left. - \frac{1}{N} \sum_l \sum_{\substack{\mu\sigma \\ (\text{occ})}} Z^\sigma_{\mu j 1 l} Z^\sigma_{\mu j 1 l+1} \right]. \qquad (19)
$$

Here, we have used the periodic boundary condition, N is the number of sites along each main chain, and (occ) means those states occupied by electrons. The density $\langle n_{jil\sigma}\rangle$ of the number of electrons and the distribution of the spin density of π electrons and unpaired electrons at the side radicals can be obtained self-consistently as

$$
\langle n_{jil\sigma}\rangle = \sum_{\substack{\mu \\ (\text{occ})}} Z^\sigma_{\mu jil} Z^{\sigma *}_{\mu jil},
$$

$$
\qquad\qquad\qquad (20)
$$

$$
\delta n_{jil} = \frac{1}{2}(\langle n_{jil\alpha}\rangle - \langle n_{jil\beta}\rangle) = \frac{1}{2}\left(\sum_{\substack{\mu \\ (\text{occ})}} |Z^\alpha_{\mu jil}|^2 - |Z^\beta_{\mu jil}|^2 \right).
$$

The energy eigenvalue ε^σ_μ, and the expansion coefficients $Z^\sigma_{\mu jil}$ can be obtained from Eqs. (13)–(20) self-consistently. The starting geometry in the iterative optimization process is usually the one with $y_{jl} = 0$ and $\langle n_{jil\alpha}\rangle = \langle n_{jil\beta}\rangle = 1/2$. The stability of the optimized geometry is always tested by using another starting configuration and performing the optimization once again. A set of solutions is reached, independent of the starting configuration. The criterion for terminating the optimization is that the differences between two successive iterations be less than 10^{-5} for the dimerization and spin density.

III. RESULTS AND DISCUSSIONS

We consider two neighboring chains as shown in Fig. 1. Each chain contains 40 carbon atoms each with a π electron. The side radicals each with an unpaired electron connect with the even carbon atoms. From Eqs. (12)–(16), we know that the eigenvalue equations are unsymmetrical about spin owing to the Hubbard electron-electron repulsion. So in this system, the spin degeneracy has been lifted, and we must solve the eigenvalue equations with different spin. In order to study the ground state, we always fill the π electrons and unpaired electrons at the side radicals in the lowest possible levels in every iterative step. In the following numerical calculations, we assume the parameters $\lambda = 0.4$, $u = 1.0$, and $t_1 = 0.9$.

First, we discuss the energy levels of the π electrons and the unpaired electrons at the side radicals, and the stability of the ferromagnetic ground state of the system. Figures 2(a) and 2(b) show the energy spectra without and with interchain coupling, respectively. If we neglect the interchain coupling, the electron energy spectra contain three down-spin energy bands and three up-spin energy bands. Each energy band contains 40 energy levels that are twofold degenerate with respect to two chains. Since there are 80 π electrons on the two main chains and 40 unpaired electrons at the side radicals, the lowest two up-spin energy bands and one down-spin energy band will be filled while the higher three energy bands will be empty. So the ground state of the system is a high-spin ferromagnetic state. This result corresponds with the situation in Ref. 12. When there exists interchain coupling, the degeneracy of energy levels with respect to different chains is lifted. This situation is shown in Fig. 2(b) for $t_2 = 0.1$, $t_3 = 0.3$, and $t_4 = 0.1$. The energy spectra contain six up-spin energy bands and six down-spin energy bands each with 20 energy levels. In this case, the ground state of the system is still a high-spin state. Figure 3 shows the total energy of the system from that without interchain interaction as a function of the interchain coupling t_2. Curves α and β correspond to $t_3 = 0.3$, $t_4 = 0.1$ and $t_3 = 0.3$, $t_4 = 0.3$, respectively. We can see clearly that the interchain coupling decreases the total energy of the system. For a definite t_3 and t_4, smaller t_2 enables the total energy to have a greater negative value. In this case, the ground state is a more stable high-spin ferromagnetic state. On the other hand, from Fig. 4, we can see that the interchain coupling decreases the energy gap. The gap reduces more rapidly with increasing of t_2 than with increasing of t_3 or t_4. Comparing curve A with curve B or comparing curve C with curve D, we find that the interchain coupling t_3 between the even sites reduces the energy gap slightly. At a critical value $t_2 = t_{2c}$, the gap disappears. The greater the values of t_3 and t_4, the smaller the critical value t_{2c}. In this case, the middle highly localized energy bands in Fig. 2 do not split off with respect to up spin and down spin, and the number of up-spin electrons occupying the energy bands is equal to the number of down-spin electrons occupying the energy bands. The ground state does not exhibit ferromagnetism. Therefore, in order to stabilize the ferromagnetic ground state, the interchain coupling should be appropriate.

Second, we discuss the distribution of spin density. Figure 5 shows spin density at different sites as a function of the

interchain interaction t_2. Curves α and β correspond to t_3 $=0.3$, $t_4=0.1$ and $t_3=0.3$, $t_4=0.3$, respectively. We find that the spin density concentrates on the side radicals, and the ferromagnetism of the high-spin ground state of the system is mainly contributed to by the unpaired electrons at the side radicals. With different interchain coupling, the spin density transfers between the main chains and the side radicals. From Figs. 5(a)–5(c), we can see obviously that for a definite t_3 and t_4, as the interchain coupling t_2 increases, the spin density at the side radicals and the even sites decreases while the spin density at the odd sites increases. This means that with increasing t_2, the spin density transfers from the side radicals and the even sites to the odd sites. Comparing curves α with β, it is shown that for a definite t_2 and t_3, with the increasing of t_4, the spin density at the side radicals and the even sites increases while the spin density at the odd sites decreases. This means that with increasing of t_4, the spin density transfers from the odd sites to the side radicals and even sites on the main chain. This result shows that the interchain coupling t_4 between the side radicals and the interchain coupling t_2 between the odd sites on the main chains have reverse effects on the transfer of spin density.

Now we discuss the dimerization of the system along each chain. Figure 6 shows the dimerization with different interchain coupling t_2. Curves α and β correspond to t_3 $=0.3$, $t_4=0.1$ and $t_3=0.3$, $t_4=0.3$, respectively. It is shown that for a definite t_3 and t_4, with the increasing of t_2, the dimerization reduces. Comparing curves α and β, we find that for a definite t_2 and t_3, with increasing of t_4, the dimerization increases.

In conclusion, we have studied an interchain coupling model for a quasi-one-dimensional organic polymer ferromagnet. It is shown that the interchain interaction makes the energy levels split off with respect to different chains. Appropriate coupling strength stabilizes the high-spin ground state of the system. However, as the interchain coupling t_2 increases to a critical value, which depends on t_3 and t_4, the energy gap disappears and the high-spin state does not exist. It is also found that in the high-spin ground state, different configurations of interchain coupling result in transfer of spin density between each main and the side radicals. The dimerization of the system varies with the interchain coupling.

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