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POLARON STATES OF THE LINEAR DIATOMIC POLYMER

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In /1/ the role of electron transfers between second-neighbour sites in the linear diatomic polymers has been studied. It was shown that their role in some AB polymers could be considerably enhanced in comparison with the polyacetylene case. Namely, the second-neighbour interactions can significantly modify an energy required to excite an AB soliton pair. In this Letter we study the influence of the second-neighbour interactions on the creation energy of polaron states in the framework of the finite-band continuum model of the diatomic polymer.

Let us consider the model Hamiltonian introduced first in /2/ and extended in /1/ in the following form:

$$H = -\sum_{n,\sigma} \sum_{l=1}^{2} t_{n,n+l}(c^{+}_{n+l,\sigma}c_{n,\sigma} + h.c.) + \alpha \sum_{n,\sigma} (-1)^{n+1} c^{+}_{n,\sigma}c_{n,\sigma} + \frac{K}{2} \sum_{n} (u_{n+1} - u_{n})^{2}, \qquad (1)$$

where $t_{n,n+1}$ denotes electron transfers between the first and second neighbours, respectively, $c^{+}_{n,\sigma}(c_{n,\sigma})$ are the creation (annihilation) operators of π-electrons with spin σ at a site n, α stands for a one-site potential, K is a harmonic spring constant and u_n are lattice displacements. The elastic interactions are restricted to the nearest-neighbour atomic cores. Also, the kinetic energy term is omitted in (1) because we are interested here in static polaron states only. The hopping matrix elements are taken in the linear forms $t_{n,n+1} = t_0 - \gamma(u_{n+1} - u_n)$ and $t_{n,n+2} = t_{2A(2B)} - \gamma_{2A(2B)}(u_{n+2} - u_n)$, where t_0 and $t_{2A(2B)}$ are the electron transfer integrals between first and second neighbours in a regular chain. The corresponding derivatives of $t_{n,n+1}$ and $t_{n,n+2}$ with respect to intersite separation a in the regular chain are denoted by $-\gamma$ and $-\gamma_{2A(2B)}$ for odd (even) sites, respectively.

The finite-band continuum equations for eigenvalues $\hat{E}_k$, eigenstate amplitudes $A_k(x)$, $B_k(x)$ in the diatomic polymer have first been derived in /3/ and can be written as

$$[E_k-(\alpha-\Delta t_{2k})]A_k(x) = -iv_{Fk}\frac{\partial B_k(x)}{\partial x} -(\varepsilon_k-i\Delta_k(x))B_k(x),$$

$$[E_k+(\alpha-\Delta t_{2k})]B_k(x) = -iv_{Fk}\frac{\partial A_k(x)}{\partial x} -(\varepsilon_k+i\Delta_k(x))A_k(x), \qquad (2)$$

together with the self-consistent gap equation

$$\Delta(x) = -\frac{4i\gamma^2 a}{K}\sum_{k,\sigma}^{occ}(A_k^*(x)B_k(x) - c.c)\cos ka. \qquad (3)$$

Here $A_k(x)$ and $B_k(x)$ are normalized by the condition $\int_{-L/2}^{L/2} dx(|A_k(x)|^2+|B_k(x)|^2) = 1$, $L=Na$ is the chain length, $\Delta(x)$ is the gap parameter, $\Delta_k(x)=\Delta(x)\cos ka$, $\varepsilon_k=2t_0\sin ka$, $\Delta t_{2k}=\Delta t\cos 2ka$, $\Delta t=t_{2B}-t_{2A}$, $v_{Fk}=v_F\cos ka$, where v_F denotes the Fermi velocity $v_F=2t_0a$. The wave vector k in (2,3) is measured relative to $k_F=\pi/2a$ and the energy $E_k=\hat{E}_k-(t_{2A}+t_{2B})\cos 2ka$.

The polaron solutions of (1,2) at $t_{2A}=t_{2B}=0$ were considered in /4/. In the general case we obtain the gap parameter $\Delta(x)$ in the usual form /5/

$$\Delta_p(x) = \Delta-K_0v_F[\tanh K_0(x+x_0)-\tanh K_0(x-x_0)], \qquad (4)$$

where $\Delta^2=\Delta_0^2-\alpha^2$ and $2\Delta_0$ is the Peierls gap in the electronic spectrum. The eigenspectrum is symmetric around E=0 and contains two localized intragap levels with energies $E=\pm\omega_0$ and two branches of conduction and valence-band states with energies $E=\pm\omega_k$. For $E=+\omega_0$ the amplitudes of a localized state are found to be

$$A_+(x)=N_0(1+i)\,\mathrm{sech}K_0(x-x_0),\quad B_+(x)=N_0'(1-i)\,\mathrm{sech}K_0(x+x_0), \qquad (5)$$

where $N_0 = [K_0(\omega_0+\alpha-\Delta t)/8\omega_0]^{1/2}$, $N_0' = [K_0(\omega_0-\alpha+\Delta t)/8\omega_0]^{1/2}$,

$\tanh 2K_0x_0 = K_0v_F/\Delta$, $K_0v_F = (\Delta_0^2-\omega_0^2)^{1/2}$, and $\Delta_0^2=\Delta^2+(\alpha-\Delta t)^2$.

For a state with $E=-\omega_0$ one obtains that $A_-(x)=(N_0'/N_0)A_+(x)$ and $B_-(x)=-(N_0/N_0')B_+(x)$.

The amplitudes of continuum states are obtained in the form

$$A_k(x)=N_k[(\omega_k-\alpha_k+\Delta_k+\varepsilon_k)-i(\omega_k-\alpha_k+\Delta_k-\varepsilon_k)+2\delta(1-i)\tanh K_0(x-x_0)],$$

$$B_k(x)=N_k[(\omega_k+\alpha_k+\Delta_k+\varepsilon_k)+i(\omega_k+\alpha_k+\Delta_k-\varepsilon_k)-2\rho(1+i)\tanh K_0(x+x_0)], \qquad (6)$$

where $N_k=\varepsilon_k[8\omega_kL(\omega_k+\Delta_k)(\varepsilon_k^2+K_0^2v_{Fk}^2-2K_0^2v_{Fk}^2/LK_0)]^{-1/2}$, $\alpha_k=\alpha-\Delta t_{2k}$,

$\delta=(1/2)K_0v_{Fk}[1-i(\omega_k-\alpha_k+\Delta_k)/\varepsilon_k]$, $\rho=(1/2)K_0v_{Fk}[1+i(\omega_k+\alpha_k+\Delta_k)/\varepsilon_k]$.

The continuum states have energies $\omega_k^2=\pm(\varepsilon_k^2+\Delta_k^2+\alpha_k^2)$. Note that at $\Delta t=0$ expressions (5,6) are reduced to those obtained in /4/.

The self-consistent condition (3) takes the form

$$[\pi/2 - K(m)E(\theta,m') - E(m)F(\theta,m') + K(m)F(\theta,m')] =$$

$$= \pi t_0(\nu_--\nu_+)[(1+y^2+l)(1-p^2)(m'^2-p^2)]^{1/2}/2\omega_0 \quad , \qquad (7)$$

where $F(\theta,m')$ and $E(\theta,m')$ are incomplete elliptic integrals of the first and second kind, respectively, $m^2=(1-z^2+2l)/(1+y^2+l)$, $m'=(1-m^2)^{1/2}$, $y=\alpha/2t_0$, $z=\Delta/2t_0$, $p=K_0v_F/2t_0$, $l=2\alpha\Delta t/4t_0^2$, $\nu_\pm$ are the occupation numbers of levels with $E=\pm\omega_0$ and the angle θ is defined as $tg\theta = p/(m'^2-p^2)^{1/2}$.

Taking into account (4-7), we obtain the polaron formation energy in the following form:

$$E_p = 4K_0v_F\{[E(m)-(1-m^2)K(m)]/m^2+(y^2+l)K(m)\}/\pi(1+y^2+l)^{1/2}$$

$$- (\alpha+\Delta t)^2(\nu_--\nu_+)p^2/\omega_0. \qquad (8)$$

Note that the polaron energy (8) depends on α and Δt. For $z^2\ll 1$, $y^2\ll 1$, $|l|\ll 1$ and $p^2\ll 1$ (the limit of the linearized continuum scheme) the result (8) is reduced to

$$E_p = \omega_0(2+\nu_+-\nu_-)+(4/\pi)[K_0v_F-\omega_0\mathrm{arctg}(K_0v_F/\omega_0)]. \qquad (9)$$

In the limit $\omega_0\to\alpha-\Delta t$ the polaron energy (9) approaches the creation energy of the kink-antikink pair (see /1/):

$$E_p = (\alpha-\Delta t)(2+\nu_+-\nu_-)+(4/\pi)[\Delta-(\alpha-\Delta t)\mathrm{arctg}(\Delta/(\alpha-\Delta t))]. \qquad (10)$$

Finally, we have calculated the polaron creation energy as a function of Δt at different values of α (see Fig.1). One can see that the consideration of electron transfers between second neighbour sites leads to the modified values of E_p. Nevertheless, these effects are less significant than those in the case of the kink-antikink pair in the diatomic polymers (see /1/).

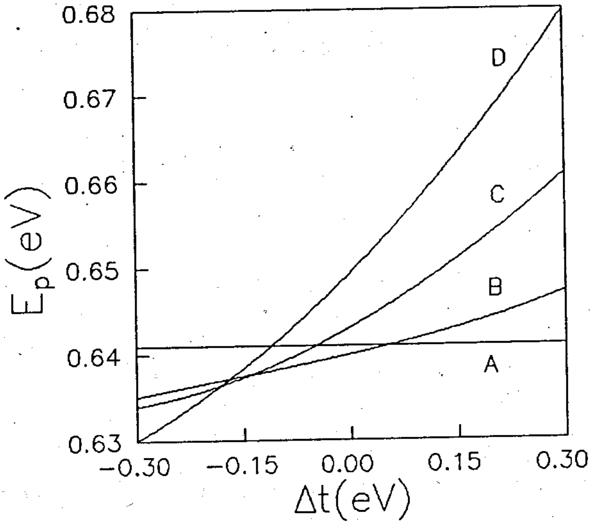

Fig.1. The polaron creation energy (8) as a function of Δt is shown. The parameter set is used: t_0=3eV, γ=80eV/nm, $K=68\times10^2$eV/nm^2. Curve A, α=0; curve B, α=0.15eV; curve C, α=0.3eV; curve D, α=0.5eV.

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