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POLARONS IN THE FINITE-BAND CONTINUUM MODEL OF DIATOMIC POLYMERS

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In the previous paper /1/ we have investigated the static polaron states in the trans-polyacetylene and polyyne models in the framework of the finite-band continuum scheme introduced for the first time in /2/. It has been shown in /1-4/ that the finite-band scheme gives more precise results in comparison with the well-known linearized continuum scheme. Here we study the physical properties of the static polaron in the diatomic polymer model /5/. The numerical calculations of polaron states in the diatomic polymer have been performed in /4/ whereas the results of the linearized continuum scheme are presented in /6/.

The finite-band continuum equations for the one-particle electronic states in the diatomic polymer have been derived first in /3/ and have the form

$$(E_k-\alpha)A_k(x) = -iv_{Fk}\frac{\partial B_k(x)}{\partial x} - (\varepsilon_k - i\Delta_k(x))B_k(x) \ ,$$
$$(E_k+\alpha)B_k(x) = -iv_{Fk}\frac{\partial A_k(x)}{\partial x} - (\varepsilon_k + i\Delta_k(x))A_k(x) \ , \qquad (1)$$

together with the self-consistent gap equation

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

Here $A_k(x)$ and $B_k(x)$ are eigenstate amplitudes 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, $\Delta_k(x)=\Delta(x)\cos ka$, $\varepsilon_k=2t_0 \sin ka$, $v_{Fk}=v_F \cos ka$, where v_F denotes the Fermi velocity $v_F=2t_0 a$. The wave vector k in (2,3) is measured relative to $k_F = \pi/2a$.

Let us consider the polaron solutions of (1,2). The gap parameter $\Delta(x)$ is obtained in the usual form /6/

$$\Delta_p(x) = \Delta_0 - K_0 v_F[\tanh K_0(x+x_0) - \tanh K_0(x-x_0)] \quad , \tag{3}$$

where $2\Delta_0$ is the Peierls gap in the electronic spectrum. As usual, the polaron distortion (3) leads to an eigenspectrum which 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

$$A_+(x) = N_0(1+i)\,\mathrm{sech} K_0(x-x_0) \quad , \quad B_+(x) = N_0'(1-i)\,\mathrm{sech} K_0(x+x_0) \quad , \tag{4}$$

where $N_0 = [K_0(\omega_0+\alpha)/8\omega_0]^{1/2}$, $N_0' = [K_0(\omega_0-\alpha)/8\omega_0]^{1/2}$, $\tanh 2K_0x_0 = K_0v_F/\Delta$, $\Delta^2= \Delta_0^2- \alpha^2$, and $K_0v_F = (\Delta_0^2 - \omega_0^2)^{1/2}$. 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

$$\begin{aligned} A_k(x) &= N_k[(\omega_k-\alpha+\Delta_k+\varepsilon_k)-i(\omega_k-\alpha+\Delta_k-\varepsilon_k)+2\delta(1-i)\tanh K_0(x-x_0)] \; , \\ B_k(x) &= N_k[(\omega_k+\alpha+\Delta_k+\varepsilon_k)+i(\omega_k+\alpha+\Delta_k-\varepsilon_k)-2\rho(1+i)\tanh K_0(x+x_0)] \; , \end{aligned} \tag{5}$$

where $N_k = \varepsilon_k[8\omega_k L(\omega_k+\Delta_k)(\varepsilon_k^2 + K_0^2v_{Fk}^2 - 2K_0^2v_{Fk}^2/LK_0)]^{-1/2}$,

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

The continuum states have energies $\omega_k^2 = \pm(\varepsilon_k^2+\Delta_k^2+\alpha^2)$.

The self-consistent condition (2) takes the form

$$[\pi/2 - K(m)E(\theta,m') - E(m)F(\theta,m') + K(m)F(\theta,m')] = \\ = \pi t_0(\nu_- - \nu_+)[(1+y^2)(1-p^2)(m'^2-p^2)]^{1/2}/2\omega_0 \quad , \tag{6}$$

where $F(\theta,m')$ and $E(\theta,m')$ are incomplete elliptic integrals of the first and second kind,respectively, $m^2=(1-z^2)/(1+y^2)$, $m'=(1-m^2)^{1/2}$, $y = \alpha/2t_0$, $z = \Delta/2t_0$, $p = K_0v_F/2t_0$, $\nu_\pm$ are the occupation numbers of levels with $E = \pm\omega_0$ and the angle θ is defined as
$\mathrm{tg}\theta = p[(1+y^2)/(y^2+z^2-p^2-p^2y^2)]^{1/2}$.

Consider now the physical characteristics of polarons. The polaron width ξ_p is defined as

$$\xi_p = 2x_0 = (1/K_0)\mathrm{arcth}(K_0v_F/\Delta). \tag{7}$$

The global charge of a polaron is obtained to be

$$Q = \int_{-L/2}^{L/2} dx\ \Delta\rho^p(x) = (2 - \nu_+ - \nu_-)|e|. \tag{8}$$

Thus, polarons have the standard charge $Q = \mp|e|$ (for $\nu_-= 2$, $\nu_+= 1$ and $\nu_-= 1$, $\nu_+= 0$, respectively) and spin $S = 1/2$.

Finally, we obtain the formation energy of polarons

$$E_p = 4K_0v_F\{[E(m)-(1-m^2)K(m)]/m^2 + y^2\Pi(\pi/2,n,m)\}/\pi(1+y^2)^{1/2} \\ + \alpha^2(\nu_+ - \nu_-)/\omega_0 , \tag{9}$$

where $\Pi(\pi/2,n,m)$ is the complete elliptic integral of the third kind and $n = -(1-p^2)$. Note that in contrast to /6/ in the finite-band scheme the polaron energy (9) depends on α. Nevertheless, for $z^2 \ll 1$ and $y^2 \ll 1$ we obtain the known results of the linearized continuum scheme /6/. In the limit $\alpha \to \omega_0$ (or, equivalently, $K_0v_F \to \Delta$) the polaron energy (9) approaches one of two kinks (see /3,4/). Moreover, from (8) we obtain that $\xi_p \to \infty$. Thus, at $\alpha = \omega_0$ the polaron state is in fact identical with a kink-antikink pair infinitely far apart. Table 1 lists the basic physical characteristics of polarons which have been calculated in the framework of the finite-band continuum scheme, numerically /4/, and in the linearized continuum scheme /6/.

Table 1. The physical characteristics of a negatively charged polaron in a diatomic polymer. The parameter set from /4/ is used: t_0= 3eV, γ = 80eV/nm, K = 68×10^2eV/nm^2, α = 0.3eV.

Model	N(sites)	Δ_0(eV)	ω_0(eV)	$2x_0$(a)	E_p(eV)
discrete	82 162 202	0.726 0.722 0.722	0.51	$\propto$12	0.647 0.645 0.645
finite band	—	0.724	0.515	12.1	0.643
linearized	—	0.706	0.499	12.6	0.636

Finally, the polaron state in a diatomic polymer is investigated in the framework of the finite-band scheme. As we expected, the finite-band scheme gives a better agreement with the numerical results as compared to the linearized continuum scheme.

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