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NONLINEAR EXCITATIONS OF A DIATOMIC POLYMER

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In our previous paper (Fedyanin and Osipov 1987), we examined the ground-state properties and soliton excitations of AB polymers within the framework of the finite band continuum scheme first proposed by Gammel (1986) for the case of polyacetylene chains. In the present paper, we study the physical characteristics of AB soliton pairs and polarons, both numerically and analytically. The aim of our paper is twofold. At first, we extend the Rice-Mele Hamiltonian (Rice and Mele 1982) by adding electron transfers between second neighbour sites since their role in some AB polymers could be considerably enhanced in comparison with the polyacetylene case. At second, we investigate numerically π-electron spectra of finite AB chains to estimate effects caused by discreteness of the lattice.

Let us consider the model Hamiltonian

$$H=-\sum_{n,\sigma}\sum_{l=1}^{2} t_{n,n+l}\left(c^{+}_{n+l,\sigma} c_{n,\sigma} + h.c \right) +$$

$$+ \alpha \sum_{n,\sigma} (-1)^{n+1} c^{+}_{n,\sigma} c_{n,\sigma} + \frac{K}{2} \sum_{n} (u_{n+1} - u_{n})^{2} \qquad (1)$$

for the linearly conjugated AB polymer, where $t_{n,n+l}$ $(n=1,2...N)$ 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 an one-site potential, K is a harmonic spring constant and u_n are lattice displacements. We note that 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 lattice configurations only. It is assumed that there is one π-electron per site.

As usual, we adopt the linear forms for hopping matrix elements

$$t_{n,n+1}=t_0-\gamma(u_{n+1}-u_n) \quad \text{and} \quad t_{n,n+2}=t_{2n}-\gamma_{2n}(u_{n+2}-u_n), \tag{2}$$

where t_0 and t_{2n} 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 $-\gamma_{2n}$. Whilst the parameters $t_0\equiv t_1^{AB}$ and $\gamma\equiv\gamma_1^{AB}$ do not depend on the site index, the hoppings t_{2n} and electron-lattice coupling constants γ_{2n} are equal to $t_2^{AA(BB)}\equiv t_{2A}(t_{2B})$ and $\gamma_2^{AA(BB)}\equiv\gamma_{2A}(\gamma_{2B})$ for odd (even) sites, respectively.

It is convenient to rewrite the Hamiltonian (1) in terms of the dimensionless bond-length changes $v_n=\gamma(u_{n+1}-u_n)/t_0$

$$H=t_0[\alpha_0\sum_{n,\sigma}(-1)^{n+1}c^+_{n,\sigma}c_{n,\sigma}+\sum_{n,\sigma}(v_n-1)(c^+_{n+1,\sigma}c_{n,\sigma}+h.c.)+$$
$$+\sum_{n,\sigma}(\hat{\gamma}_n(v_{n+1}+v_n)-\tau_n)(c^+_{n+2,\sigma}c_{n,\sigma}+h.c.)+\frac{1}{2\beta}\sum_n v_n^2], \tag{3}$$

where the dimensionless interaction parameters are defined as

$$\alpha_0=\alpha/t_0;\ \hat{\gamma}_n=\gamma_{2n}/\gamma;\ \tau_n=t_{2n}/t_0\ (\text{i.e. }\tau_n=\tau_A\text{ or }\tau_B)\ \text{and}\ \beta=\gamma^2/Kt_0 \tag{4}$$

It is well known that the ground state of (3) is the Peierls insulator possessing a spontaneous dimerization with a displacement field $u_n=(-1)^n u_0$. The ground state spectrum of (3) reads as

$$E_k=t_0[(\tau_A+\tau_B)\cos 2ka\pm 2[\tfrac{1}{4}(\alpha_0+\Delta\tau\cos 2ka)^2+\cos^2 ka+z^2\sin^2 ka]^{1/2}], \tag{5}$$

where $\Delta\tau=\tau_B-\tau_A$, $z=\Delta/2t_0=2\gamma u_0/t_0$ and $-\pi/2a<k<\pi/2a$. The spectrum (5) exhibits the Peierls gap

$$E_g=2\Delta_0=2t_0[(\alpha_0-\Delta\tau)^2+(\Delta/t_0)^2]^{1/2} \tag{6}$$

at the Fermi wave vector $k_F=\pi/2a$. The parameter z or, equivalently, the dimerization coordinate u_0, minimizes the ground state energy of the chain, i.e., it is determined as the solution of

$$1/\lambda_{eff}=\int_0^{\pi/2}\frac{\sin^2 t\,dt}{[1/4\,(\alpha_0+\Delta\tau\cos 2t)^2+\cos^2 t+z^2\sin^2 t\,]^{1/2}}, \tag{7}$$

where $\lambda_{eff}=4\gamma^2/\pi K t_0$ is the dimensionless electron-phonon coupling constant. As it follows from (6), the dimerization exists for $\Delta_0>t_0(\alpha_0-\Delta\tau)$ only. Hence, for some AB materials with α close to Δ_0 and $t_{2A}\neq t_{2B}$, the second neighbour interactions can easily suppress the dimerized structure of the ground state. In a general case, $\tau_A\neq\tau_B$, equation (7) has to be solved numerically. For $\tau_A=\tau_B$ we find

$$1/\lambda_{eff}=\frac{(1+y^2)^{1/2}}{1-z^2}[K(m)-E(m)], \tag{8}$$

where K(m) and E(m) are the complete elliptic integrals of the first and second kind, respectively, $m^2=(1-z^2)/(1+y^2)$ and $y=\alpha_0/2$. Finally, for $\Delta\tau\ll 1$ and $y\ll 1$, $\Delta\tau\ll 1$, eq 7 can be solved analytically even for $\tau_A\neq\tau_B$ and we find

$$\Delta_0=2t_0[\tfrac{1}{4}(\alpha_0-\Delta\tau)^2+z^2]^{1/2}=8t_0\exp(-1/\lambda_{eff}-1) \tag{9}$$

The charge transfer $2e^*$ between the A and B atoms becomes

$$e^*/e=\frac{1}{N}\sum_{k,\sigma}^{occ}\frac{\alpha_0+\Delta\tau\cos 2ka}{E_k}\ , \tag{10}$$

where E_k is given by (5), the sum runs over occupied states and |e| denotes the magnitude of the charge, e, on the electron.

The soliton excitations or polaron states of (3) can be found exactly for finite AB chains by direct numerical calculation or analytically taking the continuum limit of (3) which, however, provides an accurate description for $z\ll 1$ only. We shall consider here both the methods.

Let us discuss first the analytical approach. The continuum description of an AB polymer has first been reported by Rice and

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$$+ \sum_{n,\sigma} (\hat{\gamma}_n (v_{n+1} + v_n) - \tau_n)(c^+_{n+2,\sigma}\, c_{n,\sigma} + \text{h.c.}) + \frac{1}{2\beta} \sum_n v_n^2\,], \tag{3}$$

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Let us discuss first the analytical approach. The continuum description of an AB polymer has first been reported by Rice and

Mele (1982). Recently, their linearized scheme has been extended by Fedyanin and Osipov (1987) by including the electronic dispersion. Since the finite band scheme involves the Rice-Mele approach as a special case we start with finite band field equations (for details see Fedyanin and Osipov 1987) for eigenvalues E_k, eigenstate amplitudes $A_k(x)$, $B_k(x)$ and the local dimerization gap $\Delta(x)$ ($\hbar=1$)

$$(E_k-\alpha-t^A_{2k})\,A_k(x) = -iv_F(k)\,\frac{\partial B_k(x)}{\partial x} - (\varepsilon(k)-i\Delta_k(x))\,B_k(x)$$

$$(E_k+\alpha-t^B_{2k})\,B_k(x) = -iv_F(k)\,\frac{\partial A_k(x)}{\partial x} - (\varepsilon(k)+i\Delta_k(x))\,A_k(x) \tag{11}$$

and

$$\Delta(x) = -\frac{i4\gamma^2 a}{K}\sum_{k,\sigma}^{occ}(A^*_k(x)\,B_k(x) - c.c\,)\cos ka, \tag{12}$$

where the eigenvector corresponding to the eigenvalue E_k is the spinor $\psi_k(x) = (\psi^A_k(x),\psi^B_k(x)) \equiv (A_k(x)e^{-ikx},B_k(x)e^{ikx})$ normalized according to $\int_{-L/2}^{L/2}dx\,(|\psi^A_k(x)|^2+|\psi^B_k(x)|^2)=1$; $\Delta_k(x)=\Delta(x)\cos ka$; $v_F(k)=v_F\cos ka$, where v_F denotes the Fermi velocity $v_F=2ta$; $\varepsilon(k)=2t_0\sin ka$; $t^{A(B)}_{2k}=2t_{2A(2B)}\cos 2ka$ and finally, the length of the chain $L=Na\to\infty$. Only linear terms in a/ξ_0 ($\xi_0=v_F/\Delta$) are retained in (11) and (12) and, therefore, the derivatives $\gamma_{2A(2B)}$ (which appear in terms of an order of $(a/\xi_0)^2$) are absent in (11) and (12). We should note that here and hereafter the wavevector k is measured relative to $k_F=\pi/2a$.

For the ground state $\Delta(x)=$ const, the solutions of (11) and (12) are plane waves with constant amplitudes and yield the eigenvalues given by (5) with $k\to k\pm\pi/2a$. In periodic chains the topologic constraints imply that the solitons can be created from the ground state only in the form of AB soliton pairs.

Let us consider first the case of $t_{2k}\equiv t^A_{2k}=t^B_{2k}$. Since now the effect of the second neighbour hoppings results in a shift of the chemical potential only, it is convenient to introduce new energy variable $\hat{E}_k=E_k-t_{2k}$. For $\alpha<\Delta_0$ we have

$$\Delta(x)=\pm\Delta\,\mathrm{th}(x/\xi_0), \tag{13}$$

where the plus refers to an A soliton with the energy $\hat{E}_A=+\alpha$ whereas the minus to a B soliton with the energy $\hat{E}_B=-\alpha$. The continuum states have similar energies $\hat{E}_k$ as those of the dimerized chain but they are phase shifted by $\delta(k)=-\mathrm{arctg}(\Delta_k/\varepsilon_k)$.

The wave functions of single A soliton (k=0) read as

$$\psi^A_0(x)=A_0(x)=N_A\mathrm{sech}(x/\xi_0) \quad \text{and} \quad \psi^B_0(x)=B_0(x)=0, \tag{14}$$

where $N_A=[(1/2\xi_0)\,\mathrm{cth}(L/2\xi_0)]^{1/2}$. The amplitudes of continuum states ($k\neq 0$) become

$$A_k(x)=\frac{B_k(x)}{\hat{E}_k-\alpha}\,[-\varepsilon(k)+i\Delta_k\mathrm{th}(x/\xi_0)] \quad \text{and} \quad B_k(x)=(N_kL)^{-1/2}, \tag{15}$$

where $N_k=2[\hat{E}_k-\Delta^2_k\xi_0/L(\hat{E}_k-\alpha)]/(\hat{E}_k-\alpha)$. The amplitudes of single B soliton and corresponding continuum states are obtained from (14) and (15) by changing $A\to B$ and $\alpha\to-\alpha$.

The change in the local electronic density of the dimerized chain induced by the presence of the AB soliton pair is

$$\Delta\rho(x)=(\nu_A-2I_1)\,\rho^A_0(x)+(\nu_B-2I_1)\,\rho^B_0(x), \tag{16}$$

where ν_A and ν_B are occupation numbers of A and B soliton energy levels, respectively. The local deficiency in the continuum states I_1 is given by

$$I_1=\frac{1}{2(1+z)}+\frac{1}{\pi(1-z^2)}[\pi/2-K(m)E(\theta,m')-E(m)F(\theta,m')+K(m)F(\theta,m')], \tag{17}$$

where $F(\theta,m')$ and $E(\theta,m')$ are the incomplete elliptic integrals of the first and second kind, respectively, $m'=(1-m^2)^{1/2}$ and $tg\beta = \Delta(1+y^2)^{1/2}/\alpha\ (1-z^2)^{1/2}$. The charge densities $\rho_o^A(x)$ and $\rho_o^B(x)$ read as

$$\rho_o^A(x)=\frac{1}{2\xi_o}\ \mathrm{sech}^2((x-L/4)/\xi_o) \quad \text{and} \quad \rho_o^B(x)=\frac{1}{2\xi_o}\ \mathrm{sech}^2((x+L/4)/\xi_o). \tag{18}$$

As it follows from (16) the soliton charges of the AB pair are

$$Q_{A(B)} = -(\nu_\pm - 2I_\pm)|e|. \tag{19}$$

Finally, the creation energy of the AB soliton pair becomes

$$2E_{exc}(\nu_+,\nu_-)=\alpha(\nu_+-\nu_-)+\frac{4\Delta}{\pi}\{\frac{1}{m^2}[E(m)-(1-m^2)K(m)]+\frac{y^2}{(1+y^2)^{1/2}}\Pi(\pi/2,n,m)\} \tag{20}$$

where $\Pi(\pi/2,n,m)$ is the complete elliptic integral of the third kind and $n = (1-z^2)$.

Let us now discuss briefly the case of $t_{2A}\neq t_{2B}$. As relevant derivations within the finite band scheme are lengthy and do not result in close analytical formulas, we restrict our analysis in this letter only to the linearized version of equations (11) and (12). Approximating in (11) $\sin x \propto x$ and $\cos x \propto 1$ and introducing new energy variable $E_k = E_k - (t_{2A}+t_{2B})$ we arrive at the modified Rice and Mele (1982) equations

$$(E_k - (\alpha-\Delta t))\psi_A(x) = [-iv_F\nabla_x + i\Delta(x)]\ \psi_B(x)$$

$$(E_k + (\alpha-\Delta t))\psi_B(x) = [-iv_F\nabla_x - i\Delta(x)]\ \psi_A(x), \tag{21}$$

where $\Delta t = t_{2B} - t_{2A}$. Hence, changing simply $\alpha \rightarrow \alpha-\Delta t$ one can readily apply all the formulas of the Rice and Mele paper (1982). For example, the creation energy of a neutral AB soliton pair reads as

$$2E_{exc}(\nu_+,\nu_-) = (\alpha-\Delta t)(2\nu_+ - \nu_-) + \frac{4}{\pi}\ [\Delta - (\alpha-\Delta t)\,\mathrm{arctg}\,\frac{\Delta}{\alpha-\Delta t}] \tag{22}$$

From (22) it follows that the second neighbour interactions can significantly modify an energy required to excite an AB soliton pair. Similarly, changing $\alpha \rightarrow \alpha-\Delta t$ in polaron solutions of (21) (see Campbell 1986), we find that the polaron becomes unstable at $(\alpha-\Delta t)>\Delta_o/\sqrt{2}$ and decays into an AB soliton pair. Thus, the second neighbour interactions affect also the stability of the polaron states.

To investigate effects caused by discreteness of the lattice we have carried out numerical calculations on periodic chains (i.e. rings with fixed lengths) using the self consistent discrete method proposed by Shastry (1983) and applied by several authors to polyacetylene and polyyne chains and rings (Stafström and Chao 1984; Drechsler et al 1987, and Malek et al 1988). A modification of the discrete method to a diatomic polymer case is straightforward. The eigenvalue problem for a periodic chain described by the Hamiltonian (3) reads as

$$H\ |k> = E_k\ |k> \quad \text{and} \quad |k> = \sum_{n=1}^{N} \psi_k(n)\ c^\dagger_{n,\sigma}|0>, \tag{23}$$

where the eigenvalues E_k and the eigenvectors $|k>$ (the index k includes the spin index now) depend, of course, on the bond length changes $\{v_n\}$. Minimizing the total energy of the periodic chain

$$E_{tot} = \sum_{k=1}^{occ} E_k + \frac{1}{2K}\sum_{n=1}^{N} v_n^2, \tag{24}$$

under the constraint condition expressing periodic boundary conditions

$$\sum_{n=1}^{N} v_n = 0, \tag{25}$$

with respect to v_n, we arrive at the self consistent equations

$$v_n = \mu(\lambda \sum_{k=1}^{occ}[\psi_k^*(n+1)\psi_k(n)+\lambda_n\psi_k^*(n+2)\psi_k(n)+\lambda_{n+1}\psi_k^*(n+1)\psi_k(n-1)+c.c.]), \tag{26}$$

where the Lagrange multiplier λ reads as

$$\lambda = \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{occ}\left[\psi_k^*(n+1)\psi_k(n)+\hat{r}_n\psi_k^*(n+2)\psi_k(n)+\hat{r}_{n-1}\psi_k^*(n+1)\psi_k(n-1) + c.c\right] \tag{27}$$

and the index k runs over all occupied spinorbitals.

Equations (23)-(27) may be solved by an iteration procedure for the ground, AB soliton pair and polaron states, respectively, utilizing continuum theory expressions for displacements u_n as starting ansatz. The creation energy $2E_{exc}$ of an AB soliton pair and the formation energy E^P_{for} of a polaron state are $2E_{exc} = E^{AB}_{tot} - E^{DIM}_{tot}$ and $E^P_{for} = E^P_{tot} - E^{DIM}_{tot}$, where E^{AB}_{tot}, E^P_{tot} and E^{DIM}_{tot} are the relevant total energies given by (24). The ground state charge structure along the periodic chain (in ZDO approximation) reads

$$q^{DIM}(n) = \left(-\sum_{k=1}^{occ}|\psi_k^{DIM}(n)|^2 + 1\right)|e| , \tag{28}$$

where the second term in (28) describes the charge of atomic cores. The change in the charge distribution of the dimerized ring induced by the AB soliton pair, $\Delta\rho^{AB}(n)$, or by the polaron, $\Delta\rho^{P}(n)$, becomes

$$\Delta\rho^{AB(P)}(n) = -\sum_{k=1}^{occ}\left(|\psi_k^{AB(P)}(n)|^2 - |\psi_k^{DIM}(n)|^2\right)|e| , \tag{29}$$

where $\{\psi_k^{AB}(n)\}$, $\{\psi_k^{P}(n)\}$ and $\{\psi_k^{DIM}(n)\}$ are the relevant eigenvectors of (3). Typical shape of the charge distribution $\Delta\rho^{AB}(n)$ is shown in Fig 1.

The stable arrangement of single AB soliton pair on the ring is such that ring regions with positive and negative values of the order parameter $(-1)^{n+1}v_n$, respectively, have the same number of sites. Thus excited periodic chains of N = 4M+2 sites can be divided into two open chains of 2M+1 sites with soliton centres on

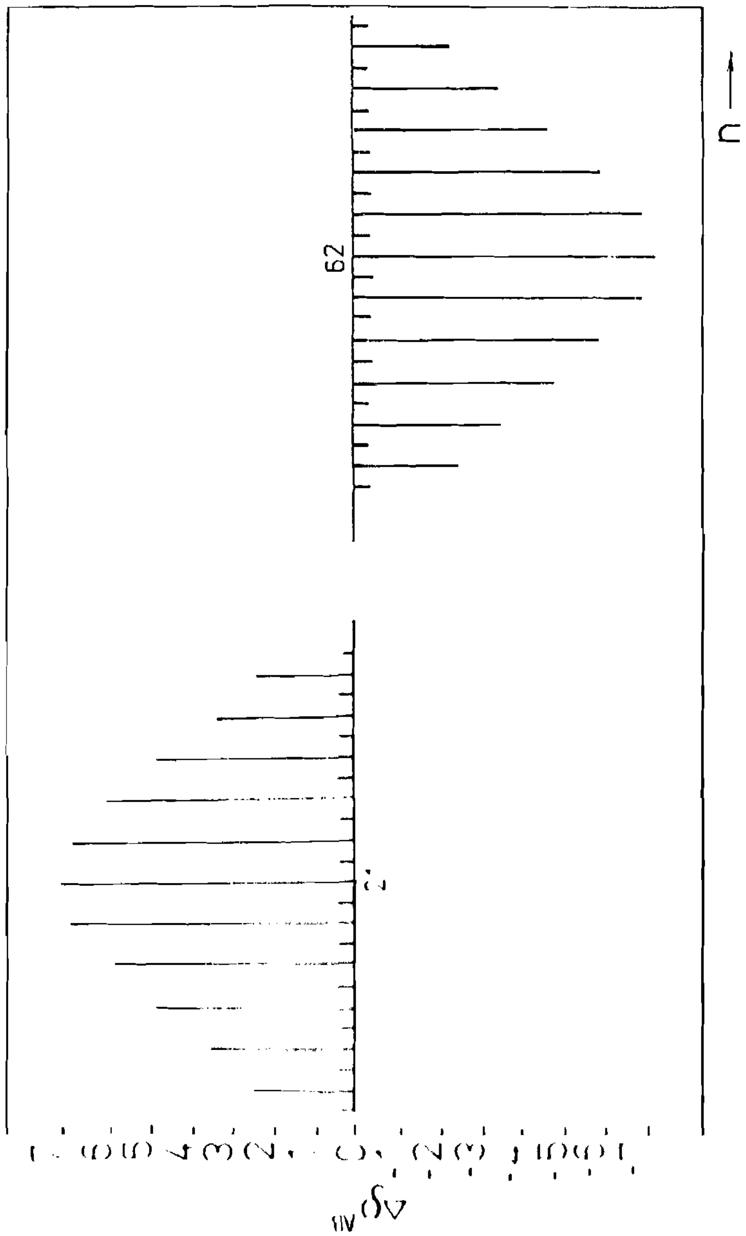

Fig 1 The charge distribution $\Delta\rho^{AB}(n)$ of an AB soliton pair (in units of 10^{-2} e) along a ring of N=82 sites. For the parameter set used see Table 1

their middle sites. For even values of M, the A soliton with energy $+\alpha$ is centered on A atom and B soliton with energy $-\alpha$, on B atom. The soliton charges Q_A and Q_B result from summing up the charge distribution $\Delta\rho^{AB}(n)$ over the corresponding regions (i.e. over A- or B-"open" chains) of the ring.

We have performed numerical calculations on the rings of N=82, 162 and 202 atoms. With the employment of the representative values t_o=3ev, K=68.6ev/Å^2, γ=8ev/Å and α=0.3ev, which yield the characteristic length $\xi_o \propto 9.1a$, we have calculated the Peierls gap $2\Delta_o$, the dimerization coordinate u_o, the soliton charges Q_A and Q_B, and the creation and formation energies of AB soliton pairs and polarons, respectively. Neglecting second neighbour transfers we have obtained results given in Tables 1 and 2. One can immediately observe the perfect agreement between the results of the finite band version of the continuum theory and the discrete model. From Tables 1 and 2 it follows also that for $a/\xi_o \ll 1$ the Rice Mele scheme is sufficiently accurate to describe well all the characteristics of the ground and excited or polaron states of AB polymers. We note there is practically no difference between the numerical results derived from the rings of 162 and 202 sites.

To verify limits of the continuum theory we have changed the spring constant to K=34.3ev/Å^2 which yields $\xi_o \propto 2.0a$. The results can be found in Table 3. In this case, of course, the linearized scheme doesn't work so well but the finite band scheme still conforms well to the results of the discrete model calculation. This is an important fact because in AB analogs of the polyyne chains one can expect solitons and polarons with very short characteristic lengths.

The decay process of the negatively charged polaron state into

Table 1. The dimerization gap parameter Δ_o(see eqs.(8) and (9) for finite band and linearized version of the continuum theory, resp.), the dimerization coordinate u_o (determined as $u_o=\Delta/4\gamma$ in the continuum model and as $u_o=-t_o v_1/2\gamma$ in the discrete model, resp), the soliton charges Q_A and Q_B, and the creation energy of the neutral AB soliton pair $2E_{exc}$ for t_o=3eV, K=68.6eV/Å^2, γ=8eV/Å, α=0.3eV, and $t_{2A}=t_{2B}=\gamma_{2A}=\gamma_{2B}=0$.

model	N(sites)	Δ_o(ev)	u_o(Å)	$Q_{A(B)}$(|e|)	$2E_{exc}$(ev)
discrete	82 162 202	0.718 0.722 0.722	0.0193 0.0204 0.0204	±0.685 ±0.722 ±0.722	0.390 0.391 0.391
finite band	--	0.724	0.0206	±0.722	0.394
linearized	—	0.706	0.0200	±0.721	0.382

Table 2. The characteristics of the negatively charged polaron. For notations and the parameter set used see Table 1

model	N(sites)	Δ_o(ev)	u_o(Å)	$Q_{A(B)}$(|e|)	E^p_{for}(ev)
discrete	82 162 202	0.726 0.722 0.722	0.0203 0.0204 0.0204	1 1 1	0.647 0.645 0.645
linearized	-	0.706	0.0200	1	0.636

Table 3. The characteristics of the neutral AB soliton pairs calculated with use of t_o=3eV, γ=8eV/Å, K=34.3eV/Å^2, α=0.3eV and $t_{2A}=t_{2B}=\gamma_{2A}=\gamma_{2B}=0$ ($\xi_o \propto 2.0a$)

model	N(sites)	Δ_o(ev)	u_o(Å)	$Q_{A(B)}$(|e|)	$2E_{exc}$(ev)
discrete	82 162 202	2.978 2.978 2.978	0.0920 0.0927 0.0927	±0.923 ±0.923 ±0.923	2.877 2.875 2.875
finite band		2.991	0.0930	±0.923	2.844
linearized		2.497	0.0775	±0.923	2.603

the charged pair of A and B solitons is shown in Fig.2. The calculation has been carried out on the ring of 162 atoms using the above mentioned parameter set with α=0.6ev and $t_{2A}=t_{2B}=0$. The polaron decays into the B soliton with the charge $Q_B=-0.367|e|$ and the A soliton with $Q_A=-0.633|e|$. The linearized theory (see Table 1) gives $\Lambda_0=0.706$ev and $\Delta=(\Lambda_0^2-\alpha^2)^{1/2}=0.372$ev, which in accord with discrete calculation, yields $Q_B=-\frac{2}{\pi}\mathrm{arctg}(\Delta/\alpha)|e|=-0.353|e|$ and $Q_A=-(1+Q_A)=-0.647|e|$.

Finally, in Fig.3 we show the effect of the second neighbour transfers on the creation energy of a neutral AB soliton pair. The calculations have been performed on the ring of 162 sites by using the parameter set with α 0.3eV and Δt varied from -0.3eV to 0.3eV. The values t_{2A} t_{2B} 0.05t_0 have been set as a centre of Δt interval. We have supposed the exponential dependence of hopping integrals t_{2A} and t_{2B} on the interatomic separation which yields γ_A $\bar{\gamma}_A$ and γ_B $\bar{\gamma}_B$ i.e. $\Delta\gamma$ $\Delta\bar{\gamma}$ γ_B γ_A (see also (4)). In accord with analytical predictions (see (22)) the calculated creation energy $2E_{sol}$ strongly depends on the value of Δt. Since $\alpha/t_0 \ll 1$ the second derivatives γ_n do not play any essential role. We note that for $\Delta t \to \alpha_0$ the localized levels are shifted to the midgap and we arrive at the well known picture of trans polyacetylene case. For $\Delta t \to (\alpha\ \Lambda_0)$ the localized levels tend to band edges and, therefore, in the polymers with α close to Λ_0, the second neighbour transfers can make the creation of AB soliton pairs impossible.

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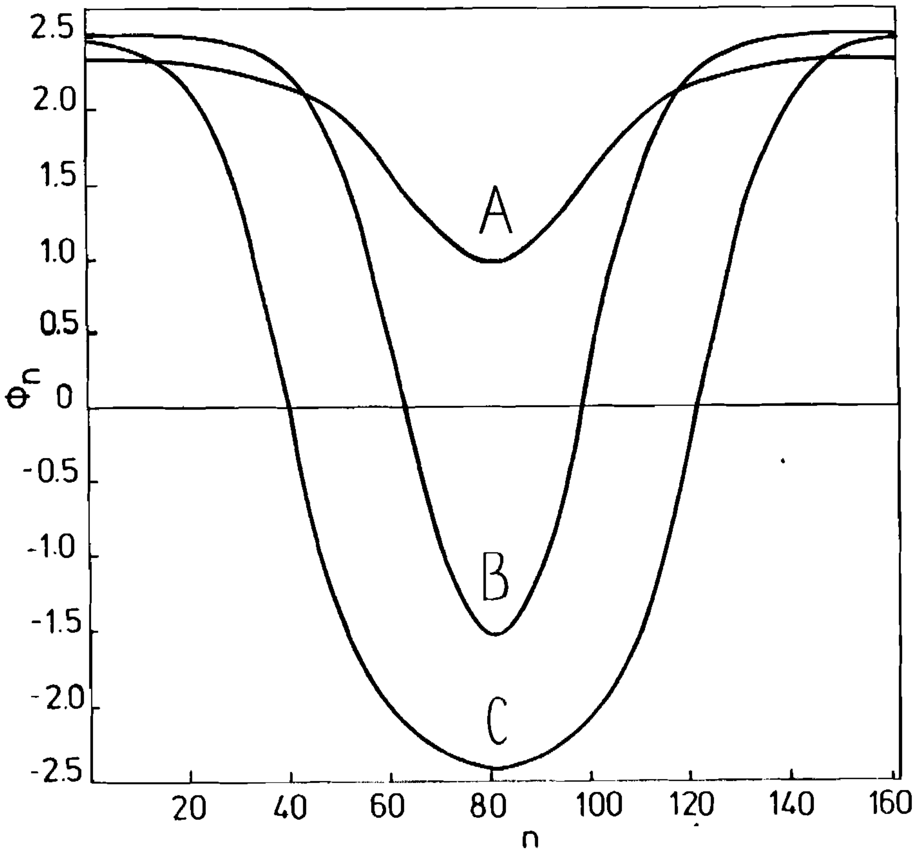

Fig.2 The decay process of a negatively charged polaron into a singly charged AB soliton pair. The order parameter $\phi_n = (-1)^{n+1} v_n t_0/\gamma$ (in units of 10^{-2} Å) is shown. The lines A, B and C display the starting ansatz, the ϕ_n after 100 iterations and the self consistent solution, respectively.

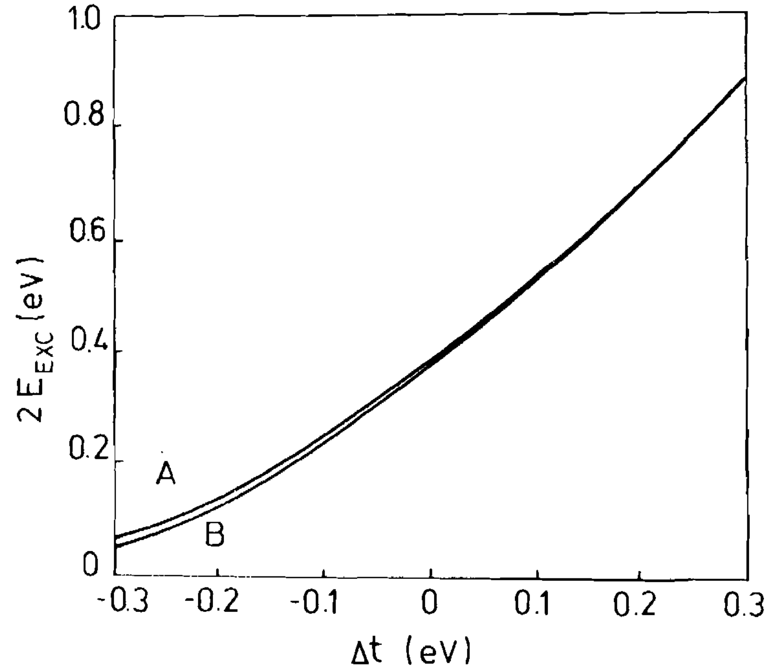

Fig. 3. The creation energy of an neutral AB soliton pair as a function of $\Delta t = t_{2B} - t_{2A}$ and $\Delta\gamma = \gamma_{2B} - \gamma_{2A}$. Analytic continuum form with $\Delta\gamma = 0$ (line A), self consistent discrete form with $\Delta t / t_0 = \Delta\gamma/\gamma$ (line B)

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Осипов В.А., Малек И., Федянин В.К. E17-88-461

Нелинейные возбуждения в двухатомном полимере

Представлены континуальный и самосогласованный дискретный анализы основного состояния, солитонной пары, а также поляронного состояния в протяженных цепочках двухатомных полимеров. Обсуждается роль эффектов, обусловленных взаимодействием вторых соседей, которая здесь существенно возрастает по сравнению со случаем полиацетилена. Вычислены пайерлсовская щель $2\Delta_0$ амплитуда димеризации u_0, заряды солитонов Q_A и Q_B, энергии рождения AB солитонной пары и полярона соответственно. Численный расчет подтверждает, что конечнозонная версия континуальной теории правильно описывает все характеристики нелинейных состояний, даже при очень коротких характеристических длинах солитонов.

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Nonlinear Excitations of a Diatomic Polymer

The continuum and self-consistent discrete analysis of the ground state, the soliton pair and polaron states of long-chain diatomic polymers is presented. The role of electron transfers between second neighbour sites is discussed and shown to be considerably enhanced in comparison with polyacetylene case. The Peierls gap $2\Delta_0$, the dimerization coordinate u_0, the soliton charges Q_A and Q_B, and the creation and formation energies of AB soliton pairs and polarons, resp., are calculated. It is verified numerically that the finite band version of the continuum theory accurately describes all the characteristics of nonlinear states under study, even when very short characteristic lengths of the inhomogeneities are considered.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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