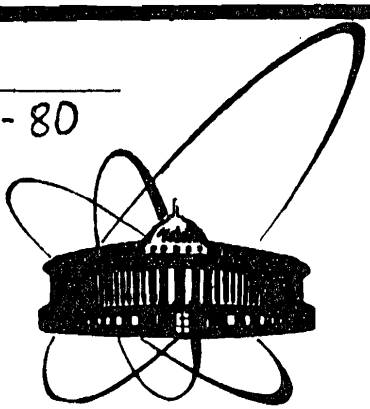

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DISCRETE EQUATIONS FOR DEFECTS IN PEIERLS SYSTEMS NEAR COMMENSURABILITY "2" WITH BROKEN ELECTRON-HOLE SYMMETRY

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I. Introduction

Many physical properties of trans-polyacetylene (PA) are explained with considerable success by the well-known Su - Schrieffer - Heeger (SSH) - model [1] and its continuum versions [2,3]. A lot of theoretical and experimental papers has been devoted in the last few years to clarify the existence and physical role of such highly nonlinear defect states as solitons and polarons (for review, see e.g. [4-6]). Recently there is an increasing interest in modifications induced by effects persisting in real PA, but neglected in the original SSH-treatment. Interchain coupling and additional long range hopping (e.g., next-nearest neighbour hopping denoted by t_2 in the following) are the simplest generalizations of the SSH-model since they do not change the single-particle character of the model. Whereas the properties of the defectless, ideal dimerized state are quite clear [7-10] the investigations of the influence of additional interactions on the defect states are much more difficult. It has been demonstrated by Maki and Baryswyl [4,9] that an interchain coupling results in a confinement of solitons (S) and antisolitons ($\bar{S}$). It is characterized by the distance $\sim 4\,\xi_0$, where $\xi_0 = 2\,at_0/\Delta_0$ is the so-called coherence length of the SSH-model. The consequences of the electron-hole (e-h) symmetry breaking [1] by, e.g., t_2 - terms are investigated very briefly in few papers [14-16]. One important result is the statement of Kivelson and Wu [16] that the presence of such terms results in a nonradiative decay of charged $S_+\,\bar{S}_-$ pairs into neutral $S_0\,\bar{S}_0$ ones which is forbidden in the SSH-model. The influence of t_2-terms on the individual characteristics of solitons or polarons remains controversal or has not been considered at all hitherto.

Stafström and Chao [14] have investigated numericaly a chain with 60 sites. According to these authors, the soliton level remains in the gap center, but the shape of the S and $\bar{S}$ wave functions change considerably. In contrast, the wave functions of the extended states remain almost unchanged.

[1] Sometimes in the quantum chemistry literature this symmetry is called also as Pariser alternancy symmetry /11/, charge-conjugation symmetry or pseudoparity /12/ (comp. /13/).

In this paper we want to give some arguments that the chosen chain length of 60 sites may possibly be too short for typical PA-parameters. Furthermore the calculation method is not optimized in order to get accurate results for sufficiently long chains.

According to Kivelson and Wu [15], the existence of t_2 - terms leads to a splitting of the creation energy of opposite charged solitons proportional to t_2 . This result is obtained by a perturbational treatment of a higher order continuum model presumably without self-consistency. Their result is understandable as a shift of the soliton level out of the gap center by the same order of magnitude.

From the general point of view the following questions arise:

i) Is the soliton level shift out of the gap center compatible with a reflectionless shape?

ii) What happens with the unique spin-charge relation since the proof of Jackiw and Schrieffer [17] is obtained by the use of the electron-hole symmetry of the density of states and the exact midgap position of a localized defect. Such questions cannot be treated in a rigorous manner by continuum models as has been demonsrated by Shastry [18] for the standard case. Finite band corrections lead to artificial irrational fractional charges since the cutoff procedures are not unique. Besides, the inspection of the changed density of states of the approximate discrete solution given by SSH demonstrates that the main change occurs near the band gap due to the presence of a soliton. Nevertheless, a finite change at the bottom of the valence band and the top of the conduction band is shown [1], too. In the presence of t_2-terms even at this extremal band edges the symmetry breaking is the strongest one. Therefore one nees for rigorous statements solutions of the discrete problem.

As a first step in this direction we obtain discrete equations using a method developed by Shastry [18] for the standard case. Equations for the evaluation of the electron energy eigenvalues and wavefunctions are derived in sec.3. In sec.4 a set of self-consistent equations is obtained where next-nearest neighbour interatomic forces are taken into account, too. In sec.2 some arguments are given for a restriction to a reduced Hamiltonian which is confined to next-nearest neighbour effects. In sec.3 we show that the perfect dimerized state satisfies these equations. In connection with various continuum models derived in sec.3 some consequences for defect states are discussed in sec.5.

2. The Model

Following our previous paper [10] we start with the general Hamiltonian in the site representation

$$H = -\sum_{l=1}^{\infty}\sum_{n,s} t_{n+l,n}\left(c^{+}_{n+l,s}\, c_{n,s} + h.c.\right) + \frac{1}{2}\sum_{l=1}^{\infty} K_l\left(u_{n+l}-u_n\right)^2 , \qquad (2.1)$$

where both the first terms in the r.h.s. describe the π -electrons. It consists of contributions from arbitrary long-range hopping processes denoted by l. The second term in the r.h.s. arises from long-range interatomic forces and the binding energy of σ - electrons. The hopping matrix elements are expanded to first order with respect to the undimerized state

$$t_{n+l,n} \approx t_l - \alpha_l\left(u_{n+l}-u_n\right), \quad l = 1,2,\ldots . \qquad (2.2)$$

Usually, the quantity t_1 in eq. (2.2) is denoted by t_0.

In order to estimate t_2, α_2 and the influence of higher order terms we use an exponential ansatz often applied in quantum chemistry literature, e.g. [18-21], or in exactly solvable Peierls model [22-24] for l=1

$$t_{n+l,n} \approx t_0 \exp\left[-\frac{\alpha_H}{t_0}\left(|\vec{R}_n - \vec{R}_{n+l}| - R_0\right)\right] , \qquad (2.3)$$

where $\vec{R}_l$ desoribe the position of the l^{th} atom. From the physical point of view such a behaviour can be expected if the long-range hopping constants are very small. Otherwise, orthogonalization corrections due to the nonorthogonality of molecular orbitals give rise to an osoillating behaviour of the long-range tails of the Wannier functions which can reault in a markable difference from the simple form (2.3) at large distances. Keeping in mind these considerations, one can estimate the magnitude of the long-range hopping integrals by making use of recent information (see below).

For this purpose we consider a zig- zag PA-ohain with 120^0-bond angles and a mean carbon-carbon distance $R_0 = 2a/\sqrt{3} \approx 1.4$ Å . In particular, the relations

$$t_{2n}/t_0 \approx \exp\left[-\frac{\alpha_H R_0}{t_0}\left(n\sqrt{3}-1\right)\right] , \quad l = 2n = 2,4,\ldots , \qquad (2.4)$$

and

$$t_{2n+1}/t_0 \approx \exp\left[-\frac{\alpha_H R_0}{t_0}\left(\sqrt{3n(n+1)+1}-1\right)\right], \quad L = 2n+1 = 1,3,\ldots, \tag{2.5}$$

are obtained from (2.3).

Equation (2.4) can be used to estimate the value of α_H from the experimentally observed dispersion of the lower $\pi-\pi^*$ interband transition edge. From the electron loss data of Fink and Leising /25/ for highly oriented PA, we deduced in /10/ $|t_2|/t_0 \approx 0.05$. Furthermore, in /19/ for the whole $\pi-\pi^*$ bandwidth $4t_0 \approx 12.8$ eV and the Peierls gap parameter $E_g = 8\alpha_{SSH} u_0 \approx 1.8$ eV were obtained. Using the relation $\alpha_{SSH} = (\sqrt{3}/2)\alpha_H$ /4/ we get from (2.4) (in units of eV/Å)

$$\alpha_{SSH} = 0.845\, t_0 \ln(t_0/t_2) \approx 8.097\,eV/Å \tag{2.6}$$

(for the value $t_2/t_0 \approx 0.1$ obtained from a bandstructure fit by Springborg /10/ , one has $\alpha_{SSH} \approx 6.2$ eV/Å, a considerably smaller value). The value of eq. (2.6) is in surprisingly excellent agreement with the estimates $\alpha_{SSH} \approx 7 \ldots 9$ eV/Å by other authors /4/ who fitted, e.g., Raman experiments, which leads to the experimental observed dimerization amplitude $u_0 \approx 0.026$Å or $Y_H^{(0)} = \sqrt{3}\, u_0 \approx 0.048$Å . These values agree with those of Fincher et al. /26/ $Y_H^{(0)} \approx 0.05$Å being obtained by X-ray diffraction and NMR nutation data. From eq. (2.5) we get $t_3/t_0 \approx 1.19\ 10^{-3}$ or $5.6\ 10^{-3}$ for $t_2/t_0 \approx 0.1$. Therefore, long-range hopping beyond the next-nearest neighbours can be neglected. All symmetry breaking effects are already taken into account by t_2 - terms and higher order terms cause only small renormalizations. In particular, the renormalization of the tight-binding band width $(4t_0)$

$$W = 4t_0\left[1+\sum_{m=1}^{\infty}\left(\frac{t_{2m}}{t_0}\right)^{\frac{\sqrt{3m^2+3m+1}-1}{\sqrt{3}-1}}\right] \approx 4t_0\left(1+\frac{t_3}{t_0}\right) \tag{2.7}$$

is of the order 10^{-3}. Analogously, the renormalization of the Peierls gap is of the same order

$$E_g \approx 8\,\alpha_{SSH}\, u_0\,(1 - t_3/t_0). \tag{2.8}$$

The linear expansion coefficients of eq. (2.2) are estimated by

$$\dot{\alpha}_\ell \approx (t_\ell/t_0)\alpha_1 \equiv (t_\ell/t_0)\alpha_{SSH} \tag{2.9}$$

According to the papers of Harrison /27,28/ and Weber /29/ , an exponential behaviour is expected for the interatomic forces in semiconductors, too . However, due to the zig-zag geometry of the PA-chain and the strong anisotropic dependence of the σ -bonding the interatomic forces are expected to vanish even faster than the electron hopping integrals with increasing distances. Therefore, we restriot ourselves to the nextnearest neighbour interaction K_2 and $K_1 \gg K_2$. The reduced Hamiltonian is rewritten with high accuracy as

$$H = H_{el} + H_{lat} , \tag{2.10}$$

$$H_{el} = -\sum_{i,s}\left[(1-v_i)(c^+_{i+1,s}\,c_{i,s} + h.c.) + (\tau - \alpha(v_{i+1}+v_i))(c^+_{i+2,s}\,c_{i,s} + h.c.)\right], \tag{2.11}$$

$$H_{lat} = \frac{1}{2\gamma_1}\sum_i v_i^2 + \frac{1}{2\gamma_2}\sum_i (v_{i+1}+v_i)^2 , \tag{2.12}$$

where dimensionless notation is introduced:

$$v_i = \frac{\alpha_1}{t_0}(u_{i+1}-u_i) , \quad \gamma_1 = \frac{\alpha_1^2}{K_1 t_0} \equiv \gamma , \tag{2.13}$$

and

$$\tau = t_2/t_0 , \quad \alpha = \alpha_2/\alpha_1 \approx \tau , \quad \gamma_2 = \frac{\alpha_1^2}{K_2 t_0} . \tag{2.14}$$

3. The Electronic Eigenvalue Equations

In order to derive discrete equations for the electron energies and wave functions it is convenient to impose periodic boundary conditions

$$c_{m+N} \equiv c_m , \quad u_{m+N} \equiv u_m , \quad 1 \le m \le N, \tag{3.1}$$

where N is the number of sites of the chain being under consideration. Introducing Fermion eigenstates for a given lattice configuration $\{u_i\}$ or $\{v_i\}$ by

$$|\Psi_\mu\rangle = \sum_m \Psi_\mu(m)\, c_m^+ |0\rangle , \tag{3.2}$$

where $|0\rangle$ denotes the vacuum state. The difference equations are obtained in the adiabatic limit from

$$H_{el}|\Psi_\mu\rangle = \varepsilon_\mu|\Psi_\mu\rangle \,, \tag{3.3}$$

by using eq. (2.10..2.14, 3.1...3.2) the anticommutation relations for the c_i and c_i^+ operators, the completeness of $c_m^+|0\rangle$ in the Fock space and $c_m|0\rangle = 0$, respectively.

We obtain

$$\begin{aligned}\varepsilon_\mu \Psi_\mu(m) = \\ = (v_{m-1}-1)\Psi_\mu(m-1) + (v_m - 1)\Psi_\mu(m+1) + \\ + [\alpha(v_{m+1}+v_m)-\tau]\Psi_\mu(m+2) + \\ + [\alpha(v_{m-1}+v_{m-2})-\tau]\Psi_\mu(m-2)\end{aligned} \tag{3.4}$$

The amplitudes obey orthonormality and completeness relations

$$\sum_m \Psi_\mu^*(m)\Psi_{\mu'}(m) = \delta_{\mu,\mu'} \,, \quad \sum_\mu \Psi_\mu^*(i)\Psi_\mu(j) = \delta_{i,j} \tag{3.5}$$

It is convenient to remove a rapidly varying phase factor from the amplitudes and to introduce a two component (spinor-) notation. For our purpose we do not take the usual left- and right-going waves (e.g., u,v in the notation of /3/) but use an odd and even site representation

$$a_n \equiv (-1)^n \Psi_\mu(2n) \,, \quad b_n \equiv (-1)^n \Psi_\mu(2n-1) \,, \tag{3.6}$$

$$\omega_n \equiv v_{2n} \,, \quad \bar\omega_n \equiv -v_{2n-1} \,. \tag{3.7}$$

In this notation eq. (3.4) can be rewritten as

$$\begin{aligned}\varepsilon_\mu a_n - a_{n+1}[\tau+\alpha(\bar\omega_{n+1}-\omega_n)] - a_{n-1}[\tau+\alpha(\bar\omega_n-\omega_{n-1})] = \\ = b_{n+1}(1-\omega_n) - b_n(1+\bar\omega_n) \,,\end{aligned} \tag{3.8}$$

and

$$\begin{aligned}\varepsilon_\mu b_n - b_{n+1}[\tau+\alpha(\bar\omega_n-\omega_n)] - b_{n-1}[\tau+\alpha(\bar\omega_{n-1}-\omega_{n-1})] = \\ = a_{n-1}(1-\omega_{n-1}) - a_n(1-\bar\omega_n) \,.\end{aligned} \tag{3.9}$$

For the comparison of various continuum limits which may be obtained from eq. (3.8)....(3.9) with the corresponding approximations used in the literature, one has to substitute the relations connecting the different site representations in the A_+ A_- notation of Gammel /30/

$$a_n = e^{ikx}(A_+ + A_-) \,, \quad b_n = -e^{-ika}e^{ikx}(A_+ - A_-) \,, \tag{3.10}$$

and expand the shifted amplitudes and gap functions in a Taylor series keeping only low order derivations. Thereby, it is assumed that a_n, b_n, ω_n and $\bar\omega_n$ are slowly varying functions in dependence on the lattice point n. I_n the lowest order of $y = a/\xi$ (where $\xi \sim \xi_0$ is a characteristic length $\xi_0 \approx 7a$) the two-gap functions ω_n and $\bar\omega_n$ become identical. Keeping first order derivatives only for the Fermi amplitudes and neglecting first order derivatives of the gap functions due to the weak coupling regime, we get from eq. (3.8 , 3.9) the usual continuum result with the trivial effect of t_2 that the soliton level is shifted to $\varepsilon_{Loc}=2\tau$ measuring it occurs at the new position of the chemical potential. Thus in this approximation the soliton levels remain at the gap center and their wave function (for sufficiently long chain $Na \gg 2\xi$) obey the usual alternative a,b character /1/, i.e. $a_{Loc} \neq 0$, $b_{Loc} = 0$ or vice versa. Nontrivial problems arise in the next order since eq. (3.8 , 3.9) cannot be decupled. Similar problems occur in keeping finite K - values (see 3.10) in a finite band continuum approximation, as it has been proposed by T. Gammel /30/ (see 3.14) even in the first order due to a connecting term $\sim 2it_2 \, a \sin 2ka \cdot \partial A_\pm/\partial x$. Thus, in the second order expansion in the continuum limit eq. (3.8-9) has the form

$$\begin{aligned}\{\tilde\varepsilon + 2\alpha[(\omega-\bar\omega) - \gamma(\omega'+\bar\omega')]\}a' - 4\tau\gamma^2 a'' = \\ = 2\gamma b'(1-\omega) + 2\gamma^2 b'' - (\omega+\bar\omega)b \,,\end{aligned} \tag{3.11}$$

$$\{\tilde{\varepsilon} + 2\alpha[(\omega - \bar{\omega}) - \gamma(\omega' - \bar{\omega}')]\}b - 4\tau\gamma^2 b'' =$$
$$= -2\gamma a'(1-\omega) + 2\gamma^2 a'' - (\omega + \bar{\omega} - 2\gamma\omega')a \,, \qquad (3.12)$$

where

$$\tilde{\varepsilon} = \varepsilon_\mu - 2\tau \qquad (3.13)$$

and $\omega_0(x) \equiv \bar{\omega}_0(x)$ is the gap in the zeroeth order. The first order finite band continuum model equations /30/ read after the addition of the t_2-band terms

$$\hat{B}_1 \begin{pmatrix} A_+(x) \\ A_-(x) \end{pmatrix} = (\hat{B}_2 + \hat{B}_3) \begin{pmatrix} A_+(x) \\ A_-(x) \end{pmatrix} , \qquad (3.14)$$

where

$$\hat{B}_1 = \hat{1}\,(E_\mu + 2t_2(\cos 2ka + ia \sin 2ka * \partial_x)) \,, \qquad (3.15)$$

$$\hat{B}_2 = -\hat{\sigma}_2 \Delta(x)(\cos ka + ia \sin ka * \partial_x) \,, \qquad (3.16)$$

$$\hat{B}_3 = 2t_0 \hat{\sigma}_3 (\sin ka + ia \cos ka * \partial_x) \,, \qquad (3.17)$$

where $\hat{1}, \hat{\sigma}_2, \hat{\sigma}_3$ are the Pauli matrices and the wavenumber k is counted from the Fermi value $k_F = \pi/2a$. The trivial continuum limit, mentioned above, is obtained from (3.14–3.17) by setting $k = 0$. Note that eq. (3.14 – 3.17) becomes wrong in the vicinity of $k \approx k_F$, i.e. far from the gap due to the sinka-term in (3.17) which results even in the absence of the t_2-terms to fast oscillations in contradiction with the assumed soft x-dependence of the amplitudes A_+ and A_-. This is in our opinion an indication against attempts to describe in a rigorous manner finite band effects in the continuum model. Thus, we have to return to the discrete problem again.

At the end of this section we note that for the dimerized state eq. (3.8–3.9) can easily be solved by

$$a_n = (-1)^n a_k \exp(2ikn) \,,$$
$$b_n = (-1)^n b_k \exp(i(2n-1)k) \,, \qquad (3.18)$$

and

$$\omega_n = \bar{\omega}_n = V \,, \qquad (3.19)$$

which leads to the eigenvalues

$$\varepsilon_k = E_k/t_0 = 2\left\{-\tau \cos 2ka \pm \sqrt{V^2 \sin^2 ka + \cos^2 ka}\right\} , \qquad (3.20)$$

in agreement with the result of the diagonalization of the general Hamiltonian obtained in our previous paper /10/. In eq. (3.18–320) k is counted from the band center as in /1/, i.e. the gap occurs at $k = k_F$.

4. The Self-Consistency Conditions

The total energy of the Hamiltonian (2.10–2.14) is

$$E_{tot} = \sum_{\mu \in occ} \varepsilon_\mu\{V_m, V_{m+1}\} + \frac{1}{2\gamma_1}\sum_m V_m^2 + \frac{1}{2\gamma_2}\sum_m (V_{m+1} + V_m)^2 \,, \qquad (4.1)$$

where the sum index μ runs over all occupied eigenstate values. Eq. (4.1) is considered as an energy functional; its minimization with respect to the V_m results in the self-consistency equations for the two-gap functions ω_n and $\bar{\omega}_n$ introduced in (3.7). In the case of closed rings, the additional condition

$$\sum_m V_m = 0 \,, \qquad (4.2)$$

must be taken into account /18/.

From eqs. (4.1) and (3.2– 4) one obtains

$$V_j + \gamma_2^{-1}(\gamma_1^{-1} + 2\gamma_2^{-1})^{-1}(V_{j+1} + V_{j-1}) =$$
$$= (\gamma_1^{-1} + 2\gamma_2^{-1})^{-1}\Big[\lambda - \sum_{\mu \in occ}\big[(\psi_\mu^*(m+1)\psi_\mu(m) + c.c.) +$$
$$+ \alpha(\psi_\mu^*(m)\psi_\mu(m+2) + c.c.) + \alpha(\psi_\mu^*(m+1)\psi_\mu(m-1) + c.c.)\big]\Big] \qquad (4.3)$$

The long-range interatomic forces result in (4.3) in a system of N coupled self-consistent equations. For the homogeneous case ($\omega = \bar{\omega} =$ const.) (see 3.1) it can easily be shown from (4.3) that γ_2 cancels out in the equations of self-consistency. Thus, the gap does not depend on K_2, similarly as it is independent of t_2 [1]. Contrary to the inhomogeneous case, we get a system of nontrivially coupled equations. The correct magnitude of γ_2 is not known at present; it is difficult to determine γ_2 by comparison with some experiments analogously as it has been done by its electronic counterpart t_2 in /10/. However, due to the anisotropy of the σ-bonds γ_2^{-1} can be expected $\gamma_2^{-1}/\gamma_1^{-1} \ll 1$ of even higher order than $t_2/t_0 \ll 1$. Therefore, we drop γ_2^{-1} in (4.39) for the sake of simplicity and the self-consistency conditions in terms of a and b read now

$$\omega_n = \gamma\left\{\lambda + \sum_{\mu\in occ}\left[(b^*_{n+1}a_n + c.c.) + \alpha(a^*_n a_{n+1} + b_n b^*_{n+1} + c.c.)\right]\right\}, \tag{4.4}$$

$$\bar{\omega}_n = \gamma\left\{-\lambda + \sum_{\mu\in occ}\left[(a^*_n b_n + c.c.) - \alpha(a^*_n a_{n-1} + b_{n+1} b^*_n + c.c.)\right]\right\}. \tag{4.5}$$

The Lagrange multiplier λ arises from (4.2) as

$$\lambda = N^{-1}\sum_{n=1}^{N/2}\sum_{\mu\in occ}\left\{\left[a^*_n(b_n - b_{n+1}) + c.c.\right] - \alpha\left[a^*_n(a_{n+1} + a_{n-1}) + 2b^*_n b_{n+1} + c.c.\right]\right\} \tag{4.6}$$

The inspection of the r.h.s. of eq. (4.3) and (4.4) shows that the electron-hole symmetry breaking term enters into the self-consistency equations in a different form than usually. Due to the a^*a and b^*b terms, the gap functions depend even for $a_{l_\mu} = 0$, $b_{l_\mu} \neq 0$ (or vice versa) on the occupation number of the soliton level in sharp contrast to the standard situation. Therefore, the creation energy of different (occupied) defects can be expected to depend on this quantum number even without taking the Coulomb interaction into account.

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[1] Such a behaviour follows immediately from the symmetry conserved by the dimerization, i.e. the gap is purely optical in this case. Only odd numbered long-range terms are expected to contribute to the gap (comp. [10]), but their influence seems to be negligibly small (for $\iota \geq 3$).

According to Stafström and Chao /31,32/ for open chains a slightly different formalism should be applied, i.e. the elastic energy of (2.14) is replaced by

$$E_{el} = \frac{K}{2}\sum_m (u_m - u_{m+1} - C)^2,$$

where C is determined from the condition that when $u_m = 0$ for all m, H gives the ground state energy of an undistorted chain. The above mentioned calculation scheme can be generalized in order to include in a Hartree - Fock approximation some features of the electron- electron - interaction (see e.g. /32,33/ for the tight-binding case).

5. Discussion

The electronic eigenvalue equations (3.6-3.9) can be solved by an iteration procedure. Starting from a reasonable initial approximation for the gap functions ω_n and $\bar{\omega}_n$, the linear system (3.8 - 9) can be solved by diagonalization of a large but necessary finite matrix. From the obtained solution for the wave function new gap functions are calculated from the self-consistency equations. This procedure has to be continued until convergency is reached. The convergency of such a procedure was demonstrated by Stafström /24/ for a chain of 100 or 150 sites (although without t_2-terms). In the present case one has to consider in our opinion somewhat longer chains with 200 ... 250 sites in order to avoid possible artificial finite chain effects (see below) or to change the parameter set resulting in $\xi_0 < 7a$. From the general point of view the present problem is characterized by two characteristic lengths $\xi \approx \xi_0 \approx 7a$ and $\xi_0(t_0/t_2) \approx 140a$. Furthermore, from a preliminary analysis of the approximate eq. (3.14 - 17) we get that a weak confinement of soliton and antisoliton would occur if their reflectionless shape is required /34/. On the other hand it is likely that odd numbered chains ought to contain always a topological defect (compare /35/). Neglecting t_2-terms in /14/ it has been shown that there exists always an exact midgap solution at $E = 0$. The proof which is given in /14/ cannot be extended to Hamiltonians containing e - h symmetry breaking t_2-terms. We mention, e.g., the simple case of a 3-site problem where eq. (3.4) is solved analytically with the result [1]

[1] In contrast to closed rings, for open chains the charge transfer between end sites it usually forbidden, i.e. $t_{N,1} = 0$, comp eq. (2) /14/. The corresponding determinant of eq. (3.4) becomes pentadiagonal (tridiagonal in the TB approximation) in the general case.

$$E_{\pm}^{(3)} = -\frac{\tilde{t}_2}{2} \pm \sqrt{2\tilde{t}_o^2 + \tilde{t}_2^2/4} \quad , \tag{5.1}$$

$$E_o^{(3)} = \tilde{t}_2 \approx t_2 \quad , \; \tilde{t}_o > t_o \; , \; \tilde{t}_o > \tilde{t}_2 > t_2 \tag{5.2}$$

Hence, the midgap state is shifted by $\Delta E_o = 3/2\ \tilde{t}_2$ out of the gap center. Similar effects are expected for other odd-numbered finite chains, e.g. for a 5- site chain the midgap level lies approximately near

$$E_o^{(5)} \approx \frac{2\,t_{1,3}}{\left(\frac{t_{1,2}}{t_{2,3}} + 2\frac{t_{2,3}}{t_{1,2}}\right)} + O(\tau^2) \approx \frac{2}{3}\tilde{t}_{1,3} \sim \frac{2}{3}t_2 \, . \tag{5.3}$$

Comparing eqs. (5.3) and (5.2) suggests that the single soliton level is shifted from E = 0 to a value proportional to the symmetry breaking term t_2. However, its position is not universal as in the simple tight-binding case and different from the chemical potential of the infinite chain $\mu = 2t_2$. This is in our opinion a strong indication that exact midgap position is not reached at least for finite chains. The question arises what happens if the chain length tends to infinity?

From a perturbational treatment of eq. (3.11 ... 3.12) energy shifts $\tilde{\varepsilon}_{loc} \propto \tau\gamma^2$ can be obtained. The correct evaluation of the other terms is difficult since the difference $\omega - \bar{\omega}$ has to be found in agreement with the self-consistency conditions (4.4 ... 4.6). The above mentioned number reproduces the first term of the perturbation result of Kivelson and Wu [12] according to:

$$E_s^{*} - E_s^{+} = t_2\left[\frac{8}{3}\left(\frac{\Delta_o}{2t_o}\right)^2 + 0.8\left(U/2t_o\right)^2 + \dots\right] ,$$

where U denotes the Hubbard-interaction not considered here. Furthermore from the asymmetry of the corrections containing terms with $\alpha \approx \tau$ different energy shifts for solitons (s) and antisolitons ($\bar{s}$), i.e.

$$\left\{a_{loc} \neq 0 \, , \; b_{loc} \sim \tau^2 \to 0\right\} \quad \text{or} \quad \left\{b_{loc} \neq 0 \, , \; a_{loc} \sim \tau^2 \to 0\right\} ,$$

can not be excluded.

Summarizing, the energy level of topological defects is possibly somewhat shifted out of the gap center due to symmetry breaking terms. The shape of the defect is presumably only approximately of the tanh-form, i.e. it is not reflectionless in a rigorous sense. In our opinion, it means to be very interesting to clarify the influence of t_2 - terms on other physical properties of the soliton. The derived equations (3.8 - 3.9) yield to be reasonable starting points to attack questions of such kinds.

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Дискретные уравнения для дефектов в пайерлсовских системах вблизи соизмеримости "2" с нарушенной электрон-дырочной симметрией

При использовании метода, предложенного Шастри/18/, выводятся дискретные уравнения для определения электронных собственных состояний как и условия самосогласования для SSH-подобной модели /учитывая дальнодействие процессов перескока и межатомных сил/. Обсуждаются возможные последствия для солитоноподобных дефектов.

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Discrete Equations for Defects in Peierls Systems near Commensurability "2" with Broken Electron-Hole Symmetry

Following a method proposed by Shastry/18/, a discrete system of electron eigenvalue equations and self-consistency conditions for the gap parameter are derived for a SSH-like model being extended by long-range hopping and long-range interatomic forces. Possible consequences for defects as soliton-like states are discussed.

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

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