STATIONARY SOLITON STATES OBEYING TWO-COMPONENT NONLINEAR SCHRÖDINGER EQUATION

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SUMMARY: In this report we represent the results of the investigation of the localized states of few extra electrons in a deformable chain, which are described by the many-component NLSE. It is shown that in the case of two extra electrons the minimum of energy corresponds to the singlet bisoliton state. In the triplet state two electrons form two almost free solitons separated by some distance which is determined by the competition between Pauli repulsion and their mutual attraction due to the nonadiabatic interaction with the phonon subsystem.

INTRODUCTION

The concept of 'molecular soliton'[1] has been intensively used to explain various phenomena in biological physics and condensed matter physics [2-4]. In this respect there arises the question of soliton interactions in low-dimensional molecular systems. It was shown in [5,6] that in the adiabatic approximation at moderate enough values of electron-phonon interaction constant two electrosolitons with opposite spins due to their interaction with the local deformation of the chain bind in a localized bound singlet spin state called 'bisoliton'. The binding energy of such state depends both on the exchange and electron-phonon interaction constants, as well as on the velocity of the bisoliton. As it was shown in [7], in the strong nonadiabatic limit, two extra electrons with opposite spins form a bound delocalized state. The interaction of two electrosolitons with parallel spins was investigated in the zero adiabatic approximation in [8] where it was shown that the triplet bound state is unstable with respect to the decay into two solitons. Here we investigate the interaction of two extra electrons with parallel spins and the interaction of two singlet bisolitons, with account of the nonadiabaticity of the system and show that the latter effect results in the 'direct' interaction between the solitons which stabilizes the two-soliton triplet state.

1 General description of the model

Let us consider a chain of the length $\mathcal{L} = Na$ (a is the lattice constant, and we assume $N >> 1$) with few extra electrons in the conductive band. Neglecting the Coulomb repulsion between electrons, such chain can be described by the Fröhlich Hamiltonian

$$H = \sum_{\sigma,k} E(k) A^{+}_{\sigma,k} A_{\sigma,k} + \frac{1}{\sqrt{N}} \sum_{\sigma,k,q} \chi(q) A^{+}_{\sigma,k} A_{\sigma,k-q} (b_q + b^{+}_{-q}) + \sum_q \hbar\omega_q b^{+}_q b_q. \qquad (1.1)$$

Here $A^{+}_{\sigma,k}$, $A_{\sigma,k}$ are creation and annihilation operators of the electron with spin projection σ and wave number k in the conductive band with the dispersion law $E(k)$, b^{+}_q, b_q are creation and annihilation operators of phonons with wave number q and frequency ω_q , the value $\chi(q)$ is determined by a short-range interaction of electrons with atom displacements (in a simple chain such displacements correspond to acoustic phonons). In a long-wave approximation, counting the energy from the electron band bottom, one can write

$$E(k) = \frac{\hbar^2 k^2}{2m}, \quad \omega_q = V_a|q|, \quad \chi(q) = i\chi q a \sqrt{\frac{\hbar}{2M\omega_q}} \qquad (1.2)$$

where m is the effective mass of an electron in the conductive band, $V_a = a\sqrt{w/M}$ is sound velocity in a chain, w is the elasticity coefficient, and χ is the electron-phonon interaction constant.

Consider the Schrödinger equation for the state vector of the system described by the Hamiltonian (1)

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)> = H|\Psi(t)> . \tag{1.3}$$

The operator of the total momentum of the system

$$P = \sum_{\sigma,k}\hbar k A^+_{\sigma,k}A_{\sigma,k} + \sum_q \hbar q b^+_q b_q \tag{1.4}$$

which is connected with the translation operator $T = exp(iPx/\hbar)$, commutes with the Hamiltonian (1). The energy of a stationary state depends on the eigenvalue p of the operator P , and every value of p corresponds to the movement with group velocity $V = dE(p)/dp$. We can pass to the coordinate system moving with this velocity

$$|\Psi(t)> = \exp(-iPVt/\hbar)\ |\tilde{\Psi}(t)>, \tag{1.5}$$

and rewrite the Schrödinger equation for stationary states in the moving reference frame

$$(H - VP)\ |\tilde{\Psi}> = E\ |\tilde{\Psi}> . \tag{1.6}$$

Let us look for the state vector in the form

$$|\tilde{\Psi}> = |\tilde{\Psi}_{ph}>|\tilde{\Psi}_e> = U(b_q)|\tilde{\Psi}_0>, \quad |\tilde{\Psi}_{ph}>= U|0_{ph}>, \quad |\tilde{\Psi}_0>= |\Psi_e>|0_{ph}> \tag{1.7}$$

which corresponds to the multiplicative adiabatic approximation.

The unitary operator, incoming in (1.7)

$$U = exp\left[\frac{1}{\sqrt{N}}\sum_q(\beta_q b^+_q - \beta^*_q b_q)\right] \tag{1.8}$$

describes the ground state renormalization caused by the electron-phonon interaction. Substituting (1.7) into (1.6) we find

$$\tilde{H}|\tilde{\Psi}_0>= E|\tilde{\Psi}_0> \tag{1.9}$$

where

$$\begin{aligned}\tilde{H} &= U^+(H - Vp)U \\ &= W + \sum_{k,\sigma}[[E(k) - \hbar Vk]A^+_{\sigma,k}A_{\sigma,k} + \frac{1}{N}\sum_q\chi(q)(\beta_q + \beta^+_{-q})A^+_{\sigma,k}A_{\sigma,k-q}] - \sum_q\hbar(\omega_q - Vq)b^+_q b_q \\ &+ \frac{1}{\sqrt{N}}\sum_{k,q,\sigma}\chi(q)A^+_{\sigma,k}A_{\sigma,k-q}(b_q + b^+_{-q}) + \frac{1}{\sqrt{N}}\sum_q\hbar(\omega_q - Vq)(\beta_q b^+_q + \beta^*_q b_q) ,\end{aligned} \tag{1.10}$$

and

$$W = \frac{1}{N}\sum_q\hbar(\omega_q - Vq)|\beta_q|^2. \tag{1.11}$$

With the help of the unitary transformation

$$A_{\sigma,k} = \sum_\lambda\Psi_\lambda(k)a_{\sigma,\lambda} \tag{1.12}$$

we can introduce new Fermi operators. The coefficients $\Psi_\lambda(k)$ can be chosen from the condition that the part of the operator (1.10) which is quadratic with respect to Fermi operators, is diagonal:

$$[E(k) - \hbar Vk]\Psi_\lambda(k) + \frac{1}{N}\sum_q\chi(q)(\beta_q + \beta^*_{-q})\Psi_\lambda(k - q) = E_\lambda\Psi_\lambda(k). \tag{1.13}$$

This transforms the Hamiltonian (1.10) into the form $\tilde{H} = H_0 + H_1$, where H_0 is the operator which describes the adiabatic states of the electron-phonon system,

$$H_0 = W + \sum_{\lambda,\sigma} \left[E_\lambda + \frac{1}{\sqrt{N}} \sum_q f_{\lambda\lambda}(q)(b_q + b^+_{-q}) \right] a^+_{\sigma,\lambda} a_{\sigma,\lambda}$$

$$+ \frac{1}{\sqrt{N}} \sum_q \hbar(\omega_q - Vq)(\beta_q b^+_q + \beta^*_q b_q) + \sum_q \hbar(\omega_q - Vq) b^+_q b_q \ , \tag{1.14}$$

and the operator H_1 is the nonadiabaticity operator,

$$H_1 = \frac{1}{\sqrt{N}} \sum_{\lambda \neq \lambda', q} f_{\lambda\lambda'}(q) a^+_{\sigma,\lambda} a_{\sigma,\lambda'}(b_q + b^+_{-q}). \tag{1.15}$$

Here

$$f_{\lambda\lambda'}(q) = \chi(q) \sum_k \Psi^*_\lambda(k) \Psi_{\lambda'}(k-q) \ . \tag{1.16}$$

2 Adiabatic approximation

In the zero adiabatic approximation neglecting the term H_1 of the Hamiltonian, Eq.(1.9) reads as

$$H_0|\tilde{\Psi}_0 >= E|\tilde{\Psi}_0 > . \tag{2.1}$$

The Hamiltonian (1.1) conserves the number of electrons, and the eigenstate of Eq. (2.1) with one extra electron has the form of the Davydov's soliton [9]. In [10] it was shown that the nonadiabaticity is not important when the inequality $Jg^2 > \hbar\omega(q = ga)$ takes place, which is equivalent to the following inequality

$$\chi^2 > w\hbar V_a/a. \tag{2.2}$$

Here

$$J = \frac{\hbar^2}{2ma^2}, \qquad g = \frac{\chi^2}{2Jw}. \tag{2.3}$$

We shall assume the condition (2.2) being fulfilled and consider zero adiabatic approximation (2.1).

2.1 Two-particle states

In the presence of two extra electrons in a chain, the eigenstate of the Schrödinger equation (2.1) can be written in the general form as

$$|\Psi_0 >= a^+_{\alpha\sigma} a^+_{\alpha'\sigma'}|0 > . \tag{2.4}$$

For the sake of simplicity we shall consider the states with zero total momentum. Substituting (2.4) into Eq.(2.1), we get

$$H_0|\Psi_0 >= \left\{ W + E_1 + E_2 + \frac{1}{\sqrt{N}} \sum_q \left[[\hbar\omega_q \beta^*_q + f_{11}(q) + f_{22}(q)] b_q + h.c. \right] \right\} |\Psi_0 >, \tag{2.5}$$

from where we conclude that the state (2.4) is the eigenstate with the energy

$$E = W + E_1 + E_2, \tag{2.6}$$

provided the equality fulfills

$$\beta_q = \beta_{12}(q) = -\frac{\chi^*(q)}{\hbar\omega_q} \left[\sum_k \Psi^*_1(k)\Psi_1(k-q) + \sum_k \Psi^*_2(k)\Psi_2(k-q) \right] . \tag{2.7}$$

We shall look for the solution of Eq.(1.13) with account of (2.7) at small values of k, and use the long-wave approximation (1.2) when the transformation is valid

$$\Psi_\lambda(x) = \frac{1}{\sqrt{L}} \sum_k \Psi_\lambda(k) \exp{(ikxa)}, \tag{2.8}$$

Now Eq. (1.13) written in terms of the continuous variable x, takes the form

$$-\frac{\hbar^2}{2ma^2}\frac{d^2\Psi_\lambda}{dx^2} + U(x)\Psi_\lambda = E_\lambda \Psi_\lambda, \tag{2.9}$$

which coincides with the Schrödinger equation for an electron in the potential U(x) created by the lattice deformation. Accounting for (2.8) and (2.7), we find

$$U(x) = \frac{1}{N}\sum_q \chi(q)[\beta_{12}(q) + \beta^*_{12}(-q)] \exp{(-iqxa)} \;\; = \;\; - \frac{\chi^2}{w}(|\Psi_1|^2 + |\Psi_2|^2). \tag{2.10}$$

Thus, the self-consistent states of electrons and lattice deformation obey the stationary two-component nonlinear Schrödinger equations [11,12]

$$\frac{d^2\Psi_1}{dx^2} = \mu_1^2\Psi_1 - 2g(\Psi_1^2 + \Psi_2^2)\Psi_1,$$

$$\frac{d^2\Psi_2}{dx^2} = \mu_2^2\Psi_2 - 2g(\Psi_1^2 + \Psi_2^2)\Psi_2. \tag{2.11}$$

Here we have taken into account that the bound states of electrons in the deformation potential U(x) correspond to real wave functions, and introduced the notations

$$E_i \;=\; -\frac{\hbar^2\mu_i^2}{2ma^2}, \quad i = 1,2. \tag{2.12}$$

The parameter g is determined in Eq.(2.3).

The system of Eqs. (2.11) admits the solution $\Psi_1 = \Psi_2$ which corresponds to the lowest energy

$$E_{bs} = -\frac{2}{3}Jg^2, \qquad \mu = g \tag{2.13}$$

and describes the bisoliton [5,6]. In the physical system considered here, this solution has the sense only in the case of opposite spins of electrons in the initial state, i.e., when the inequality $\sigma \neq \sigma'$ takes place in (2.4).

The system (2.11) can be solved using the inverse scattering transformation [11] for the two-soliton state, as it was done in [6], or, since it belongs to the Liouville-type class [13], using the method of quadraturs, as it was done in [8]. This solution reads as follows

$$\Psi_1 \;=\; \sqrt{\frac{\mu_1^2 - \mu_2^2}{g}}\;\frac{\mu_1\;\cosh\phi_2}{S}, \qquad \Psi_2 \;=\; \sqrt{\frac{\mu_1^2 - \mu_2^2}{g}}\;\frac{\mu_2\;\sinh\phi_1}{S}, \tag{2.14}$$

where

$$S \;=\; \mu_1\;\cosh\phi_1\cosh\phi_2 \;-\; \mu_2\sinh\phi_1\sinh\phi_2, \;\; \phi_1 \;=\; \mu_1(x+\lambda), \;\; \phi_2 \;=\; \mu_2(x-\lambda). \tag{2.15}$$

and λ is the constant of integration. Introducing the operator of the number of electrons on the n-th site of the chain

$$N_{n,\sigma} \;=\; A^+_{n,\sigma}A_{n,\sigma}$$

we can calculate the electron density distribution

$$\rho \;=\; \sum_\sigma < \Psi|A^+_{n,\sigma}A_{n,\sigma}|\Psi > \;=\; \Psi_1^2(na) + \Psi_2^2(na)$$

$$= \frac{\mu_1^2 - \mu_2^2}{g} \, \frac{\mu_1^2 \cosh^2 \phi_1 + \mu_2^2 \sinh^2 \phi_2}{S^2}. \tag{2.16}$$

The energy of the corresponding state, according to (2.6), equals

$$E = -\frac{\hbar^2 \mu_i^2}{2ma^2} - \frac{\hbar^2 \mu_2^2}{2ma^2} + \frac{\hbar^2 g}{2ma^2} \int_{-L/2}^{L/2} (\Psi_1^2 + \Psi_2^2)^2 \, dx$$

$$= -J(\mu_1^2 + \mu_2^2) + \frac{4J}{3g}(\mu_1^3 + \mu_2^3). \tag{2.17}$$

The parameters μ_1 and μ_2 which determine the energies of bound states, should be found from the normalization conditions

$$\int_{-L/2}^{L/2} \Psi_i^2 dx = 1,$$

and, hence, depend on the length of the chain. At long enough chain when $L \to \infty$ the normalization conditions result in $\mu_1, \mu_2 \to \mu = g/2$. Let $\mu_1 = \mu + \Delta$, $\mu_2 = \mu - \Delta$. Then at infinitely small Δ we get

$$\Psi_1 = \frac{\mu}{\sqrt{2g \cosh(2\mu\lambda)}} \left[\frac{e^{-\mu\lambda}}{\cosh[\mu(x-R)]} + \frac{e^{\mu\lambda}}{\cosh[\mu(x+R)]} \right],$$

$$\Psi_2 = \frac{\mu}{\sqrt{2g \cosh(2\mu\lambda)}} \left[\frac{e^{\mu\lambda}}{\cosh[\mu(x-R)]} - \frac{e^{-\mu\lambda}}{\cosh[\mu(x+R)]} \right] \tag{2.18}$$

from where it follows

$$\rho = \Psi_1^2 + \Psi_2^2 = \frac{\mu^2}{g} \left[\cosh^{-2}[\mu(x-R)] + \cosh^{-2}[\mu(x+R)] \right], \tag{2.19}$$

where

$$R = \frac{1}{2\mu} \ln \frac{2\mu \cosh(2\mu\lambda)}{\Delta} \to \infty \quad \text{at} \quad \Delta \to 0. \tag{2.20}$$

The integration constant λ as it follows from Eq.(2.25), does not income into ρ but it determines the electron state. At $\lambda = 0$ the electron state is absolutely collectivized and both electrons participate in the formation of the collective state with equal probabilities, while at $\lambda \neq 0$ the symmetry is broken and at large enough value of λ functions Ψ_1 and Ψ_2 describe individual solitons respectively. The value of μ determined from the normalization condition, equals $\mu = g/2$, and two electrons have the energy

$$E = -\frac{1}{6} J g^2 + 2Jg^2 \cosh^2(g\lambda) \exp(-2gR) \tag{2.21}$$

from where it follows that there is the repulsion between solitons, caused by the exponentially decreasing force

$$F = \frac{\partial E}{\partial R} \propto \exp(-2gR). \tag{2.22}$$

This is confirmed by the numeric calculations of the wave functions (2.14) (see also [8]), from which it follows that in the long enough chain the two solitons are repelled from one another so that the distance between them exceeds their size. The integration constant λ characterizes the level of the hybridization of electrons in the bound state. At $|\lambda| \geq 5$ the electrons with parallel spins form the unbound state, and their wavefunctions can be described as independent free solitons.

2.2 Four-particle states

In the case when there are four extra electrons in a chain the eigenstate can be chosen in the form

$$|\Psi_4> = \; A^+_{1,\uparrow}A^+_{1,\downarrow}A^+_{2,\uparrow}A^+_{2,\downarrow} \; |0> \tag{2.23}$$

and calculations similar to given in Section 2.1, show that the equality takes place

$$H_0 \; |\Psi_4> = \; \left[W + 2E_1 + 2E_2 + \frac{1}{\sqrt{N}} \sum_q [\hbar\omega_q\beta^*_q + 2(f_{11}(q) + f_{22}(q))b_q + h.c.] \right] |\Psi_4> \tag{2.24}$$

where

$$\hbar\omega_q\beta_q \;\; = \;\; -2 \; [f_{11}(q) + f_{22}(q)]. \tag{2.25}$$

This leads to the results similar to the one obtained above with the substitution $g \; \to \; G = 2g$. The energy corresponding to this state, is

$$E \;\; = \;\; 2E_{bs} \;\; + \;\; 8Jg^2 \cosh^2{(2g\lambda)} \exp{(-4gR)} \tag{2.26}$$

where E_{bs} and R are determined in (2.13) and (2.20), respectively.

This means that in the zero adiabatic approximation there is the exponentially decreasing with distance repulsion between two bisolitons, due to which the bisolitons are separated by the distance as maximum as possible for the given chain length.

3 The account of nonadiabatic terms

Below we shall show that the account of the nonadiabatic term H_1 (1.15) of the Hamiltonian results in additional direct interaction between the two solitons via the phonon field which stabilizes the two-soliton solution. We shall consider only the triplet state of two extra electrons since this result can be easily generalized for the case of few bisolitons, as it has been shown above. We shall consider the nonadiabatic term of the Hamiltonian H_1 determined in Eq. (1.15) as the perturbation. One can write the first order energy correction in the form

$$\Delta E \;\; = < \Psi_0 \mid H_1 \; \frac{1}{E - H_0} \;\; H_1 \mid \Psi_0 >, \tag{3.1}$$

where the operator notation is used

$$\frac{1}{E - H_0} \;\; = \;\; \lim_{\epsilon \to 0} \; \Re\frac{1}{i} \int_0^\infty \exp{\{i(E - H_0 + i\epsilon)\tau\}} \; d\tau. \tag{3.2}$$

Here the wavefunction of the triplet state and the corresponding energy in the zero adiabatic approximation are determined in Eqs. (2.4), (2.6), respectively. Notice, that the sum in (1.15) should be taken over all states, including the bound states $\lambda = 1, 2$, and continuous spectrum characterized by the wave number κ.

The expression (3.1) can be simplified with respect to the electron operators and transformed to the following one

$$\Delta E \;\; = \;\; \lim_{\epsilon \to 0} \; \Re\frac{1}{i} \int_0^\infty \;\; d\tau \; M \;\; \exp{\{i(E + i\epsilon)\tau\}}, \tag{3.3}$$

where

$$M \;\; = \;\; \sum_j \frac{1}{N} \; \sum_{\kappa,q,q'} \;\; f_{j,\kappa}(q')f^*_{j,\kappa}(q)M_{ph}(q,q') \;\; \exp{\{-i(W + E_{i\neq j} + E_\kappa)\tau\}}, \tag{3.4}$$

$$M_{ph}(q,q') \;\; = \;\; {}_{ph} < 0|b_{q'}e^{-iV_j\tau}b^+_q|0>_{ph}, \tag{3.5}$$

Here V_j is the part of the Hamiltonian (1.10) which contains the phonon operators only, namely,

$$V_j \;\; = \;\; \sum_q \;\; \left[\hbar\omega_q b^+_q b_q \;\; - \;\; \frac{1}{\sqrt{N}} [\alpha^*_j(q)b^+_q + \alpha_j(q)b_q] \right], \tag{3.6}$$

where

$$\alpha_j(q) \;=\; f_{j,j}(q) \;-\; f_{\kappa,\kappa}(q). \tag{3.7}$$

Substituting Eq. (3.6) into (3.5), we get

$$M_{ph}(q,q') \;=\; e^{iW_j\tau+g(\tau)}\left[e^{-i\hbar\omega_{q'}\tau}\delta_{qq'} \;+\; \frac{\alpha_j^*(q')}{N\hbar\omega_{q'}}\left(1 \;-\; e^{-i\hbar\omega_{q'}\tau}\right)\frac{\alpha_j(q)}{\hbar\omega_q}\left(1 \;-\; e^{-i\hbar\omega_q\tau}\right)\right] \tag{3.8}$$

where

$$W_j \;=\; \frac{1}{N}\sum_q \frac{|\alpha_j(q)|^2}{\hbar\omega_q}, \quad g(\tau) \;=\; \frac{1}{N}\sum_q \frac{|\alpha_j(q)|^2}{(\hbar\omega_q)^2}\left(e^{-i\hbar\omega_q\tau} \;-\; 1\right). \tag{3.9}$$

Now we can rewrite the energy correction in the following form:

$$\Delta E \;=\; \frac{1}{N}\sum_{j,\kappa}\left\{\sum_q |f_{j\kappa}(q)|^2\Phi_j(\Delta_{j\kappa}+\hbar\omega_q) \;+\sum_{q'}\frac{f_{j\kappa}(q')\alpha_j^*(q')}{\hbar\omega_{q'}}\sum_q\frac{f_{j\kappa}^*(q)\alpha_j(q)}{N\hbar\omega_q}I_j\right\} \tag{3.10}$$

where the notations are used for the real parts of integrals

$$\Phi_j(z) \;=\; \Re\frac{1}{i}\int_0^\infty e^{-iz\tau}e^{g(\tau)}d\tau, \quad z \;=\; E_\kappa - E_j - W_j$$

$$I_j \;=\; \Re\frac{1}{i}\int_0^\infty d\tau\exp\left[-i(E_\kappa - E_j - W_j - i\epsilon)\tau + g(\tau)\right]\left(1 - e^{-i\hbar\omega_{q'}\tau}\right)\left(1 - e^{-i\hbar\omega_q\tau}\right) \tag{3.11}$$

To calculate the functions (3.8)-(3.9), we need to know the coefficients (3.7) determined via the functions of complete spectrum of the two-component NLSE (2.11) by the relations (1.16), (2.8). The functions corresponding to bound states are given by expressions (2.18)-(2.19). The functions of continuous spectrum, according to (2.16), can be found as the solutions of the PDE

$$\frac{d^2\psi_\kappa}{dx^2} \;=\; -\;E_\kappa\psi_\kappa \;-\; 2\,\frac{d^2}{dx^2}\,(\ln S)\psi_\kappa, \tag{3.12}$$

where the potential function S is given by expression (2.15), and, hence, read as

$$\psi_\kappa \;=\; be^{i\kappa x}\left(i\kappa \;+\; \frac{1}{2}\,\frac{d}{dx}\ln U\right) \tag{3.13}$$

where

$$U \;=\; \frac{d^2}{dx^2}\,\ln S \;=\; g(\psi_1^2 \;+\; \psi_2^2). \tag{3.14}$$

The integration constant b can be found from the normalization condition of functions (3.13):

$$b \;=\; \frac{1}{\sqrt{L(\kappa^2+\epsilon_0)}}, \quad \epsilon_0 \;=\; \frac{\mu_1^2+\mu_2^2}{2} \tag{3.15}$$

Substituting now functions (2.18), (3.13) into (1.15) and using the transformation (2.8), we find the complete set of coefficients (1.16):

$$f_{j,\kappa}(q) \;=\; -\;\frac{2iq\pi\chi(q)}{\cosh\frac{k\pi}{2\mu}\sqrt{2gL(\kappa^2+\epsilon_0)}\cosh(2\mu\lambda)}\times\begin{cases}\cosh(\mu\lambda - ikR), & j=1\\ \sinh(\mu\lambda + ikR), & j=2\end{cases} \tag{3.16}$$

$$f_{j,j}(q) = \frac{\pi q\chi(q)\cosh(2\mu\lambda \;\pm\; iqR)}{g\cosh(2\mu\lambda)\sinh\frac{q\pi}{2\mu}}, \quad j=1,2 \tag{3.17}$$

where $k = \kappa + q$. These, together with (3.7), allow us to calculate g-factor (3.9):

$$g(\tau) \;\approx\; -iW_j\tau - A_j^2\tau^2, \quad A_j^2 \;=\; \frac{1}{N}\,\sum_q |f_{jj}(q)|^2. \tag{3.18}$$

Substituting this result into the function in (3.11), we find that it is determined by the hypergeometric function $\Phi(a,b;z)$:

$$\Phi_j(z) \;=\; -\;\frac{z+W_j}{2A^2}\;e^{-\frac{(z+W_j)^2}{4A^2}}\;\Phi\left(\frac{1}{2};\frac{3}{2};\frac{(z+W_j)^2}{4A^2}\right). \tag{3.19}$$

Here

$$A^2 \;\equiv\; \frac{1}{N}\sum_q |f_{j,j}(q)|^2 \;\approx\; \frac{16\hbar\chi^2 a}{\pi M V_a g^2}\;\mu^4\;\frac{\cosh 4\mu\lambda}{\cosh^2 2\mu\lambda}\;\left(1\;+\;\frac{\sin 2\beta}{4\beta\cosh 4\mu\lambda}\right), \tag{3.20}$$

$$\beta \;=\; \frac{2\mu R}{\pi}, \tag{3.21}$$

where R is determined in Eq.(2.20).

Since the phonon part of energy W_j (see Eq. (3.9)) is small as compared with the eigenenergies of the localized states in the zero adiabatic approximation, we have

$$W_j \;\ll\; E_j, \quad z \;\approx\; E_\kappa - E_j, \tag{3.22}$$

and, hence,

$$\frac{(z+W_j)^2}{4A^2} \;\approx\; \frac{z^2}{4A^2} \;=\; \frac{g\pi^2}{2^7\gamma} \;\gg\; 1, \tag{3.23}$$

where γ is the nonadiabaticity parameter:

$$\gamma \;=\; \frac{\hbar V_a \pi}{Ja}. \tag{3.24}$$

Taking into account inequality (3.23), we find from (3.19)

$$\Phi_j(z) \;\approx\; -\;\frac{1}{z+W_j} \tag{3.25}$$

which, together with the definition (3.11), transforms the expression for energy correction (3.10) into the following one:

$$\Delta E \;=\; \sum_{j,\kappa}\left\{-\;\frac{\sum_q |f_{j\kappa}(q)|^2}{N(z+W_j)} \;+\; \frac{\sum_q \hbar\omega_q |f_{j\kappa}(q)|^2}{N(z+W_j)^2} \;-2\;\frac{|\sum_q f_{j\kappa}(q)\alpha_j(q)|^2}{N^2(z+W_j)^3}\right\}, \tag{3.26}$$

and, further,

$$\Delta E \;\approx\; -\;\frac{2m}{N\hbar^2}\;\sum_{j,\kappa,q}\;\frac{|f_{j\kappa}(q)|^2}{\mu_j^2+\kappa^2}. \tag{3.27}$$

Using now in the latter expression the explicit form of the coefficients (3.16) and changing the sum by integral over wavenumbers, we finally get:

$$\Delta E \;=\; \Delta E_1 \;+\; \Delta E_2, \tag{3.28}$$

where

$$\Delta E_1 \;=\; -\frac{\alpha}{2J\pi^2}\int_{-\infty}^{\infty}\frac{d\kappa}{(\kappa^2+\mu^2)^2}\int_{-\infty}^{\infty}\frac{|q|^3 dq}{\cosh^2\frac{\pi(\kappa+q)}{2\mu}} \;\approx\; -\;J\frac{\gamma g^3}{2^3\pi^6}, \tag{3.29}$$

$$\begin{aligned}\Delta E_2 \;&=\; -\frac{\alpha}{2J\pi^2}\int_{-\infty}^{\infty}\frac{d\kappa}{(\kappa^2+\mu^2)^2}\int_{-\infty}^{\infty}\frac{|q|^3\cos\left[2(\kappa+q)R\right]}{\cosh^2\frac{\pi(\kappa+q)}{2\mu}}\cosh\left(2\mu\lambda\right)\,dq\\ &\approx\; -\;\frac{3Jg\gamma}{(2\pi)^3\cosh\left(\lambda g\right)}\;\frac{1}{R^2}\;\left(1\;-\;\frac{1}{3}\cos\frac{2gR}{\pi}\right).\end{aligned} \tag{3.30}$$

4 Conclusion

Present considerations confirm that the lowest state of two extra electrons in a chain correspond to the singlet bisoliton. In a triplet state there is the repulsion between two electrons as well as between two bisolitons. This situation is opposite to what happens with two small bipolarons which, as it is shown in [12,13], are attracted to one another and form a bipolaron drop.

The repulsion between two (bi)solitons is partly compensated by the interaction between electrosolitons via the phonon field. The latter is described by the nonadiabatic terms of the Hamiltonian. The corresponding lowering of energy of the system consists of two parts, one of which, given by expression (3.29), is constant and small (proportional to the nonadiabaticity of the system), and another one, (3.30), depends on the distance between the solitons c.m.c., R, calculated in the zero adiabatic approximation.

Taking into account the results obtained in sections 2 and 3, we can write the total energy of a chain with two extra electrons in it within the first order perturbation accuracy (see Eqs.(2.26), (3.28)-(3.30):

$$E = -\frac{1}{6}Jg^2\left(1+\frac{3\gamma}{8\pi^6 g}\right) + 2Jg^2\frac{e^{-2gR}}{\cosh^2(\lambda g)} - \frac{3Jg\gamma}{(2\pi)^3R^2\cosh(\lambda g)}\left(1-\frac{1}{3}\cos\frac{2gR}{\pi}\right). \quad (4.1)$$

As usually, the minimization of the expression (4.1) with respect to R, which is equivalent to the solution of the equation

$$x^3 e^{-x} = B, \quad (4.2)$$

where

$$B = \frac{6g\gamma\cosh(\lambda g)}{(2\pi)^3}, \quad x = 2gR, \quad R = \frac{1}{g}\ln\frac{g\cosh(2\mu\lambda)}{\sqrt{\mu_1^2-\mu_2^2}}, \quad (4.3)$$

determines the equilibrium distance between the solitons c.m.c. The numeric solution to the latter transcendent equation is plotted on Fig.5, from where we conclude that the more is the nonadiabaticity of the system (remaining, of course, small, $B < B_{cr}$), the less is the repulsion between the two electrosolitons in the triplet state, or, respectively, between two bisolitons, and, hence, the less is the distance between the (bi)solitons c.m.c.

As a result, in the presence of N_e extra electrons in chain, the periodic lattice of bisolitons is formed in it with the distribution period $l = N/N_{bs}$, $N_{bs} = N_e/2$ [14,15] that corresponds to the many-electron solution of the Peierls-Fröhlich problem at zero temperature [15].

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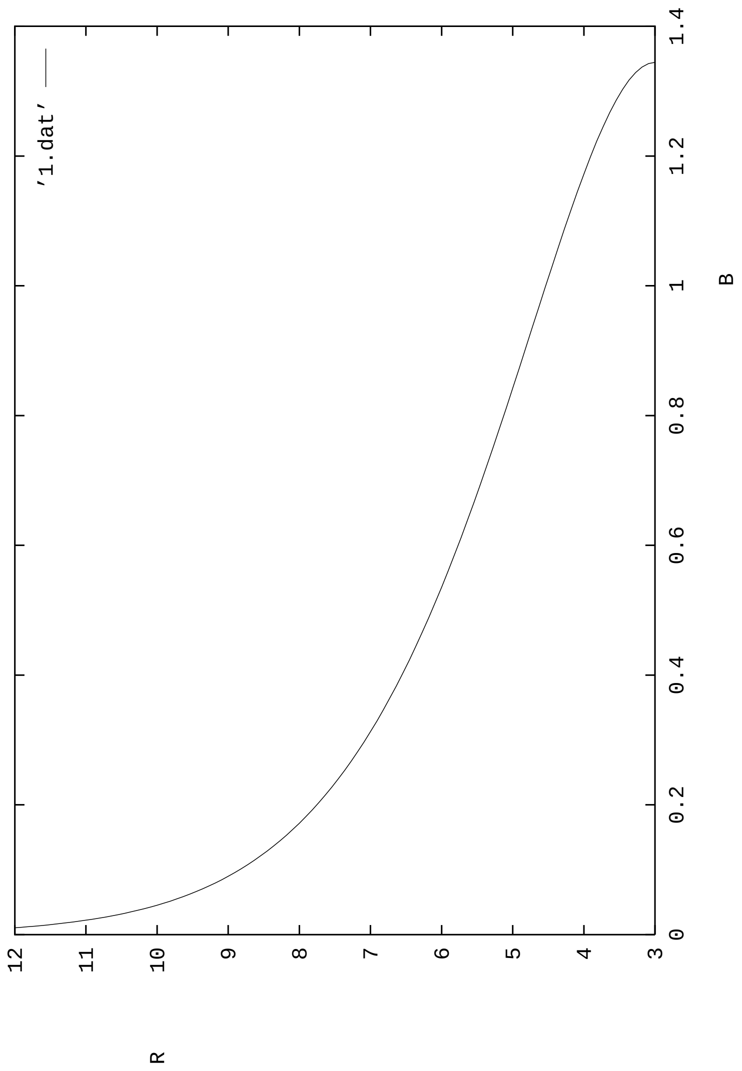

Figure 1: The dependence of the equilibrium distance between the solitons c.c.c. on the nona-diabaticity of the system.

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