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ON INTERACTION BETWEEN SOLITONS IN THE MODEL OF ORGANIC CHARGE TRANSFER SALTS

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INTRODUCTION

In the past few years the transport properties of the quasi-one-dimensional organic compounds have been extensively studied[1]. Special attention is paid to various nonlinear transport mechanisms due to solitons[2]. A number of exact classical and quantum models that have been suggested allow one to investigate the system dynamics in detail[3]. The organic salts like TTF-TCNQ have two subsystems: donor and acceptor chains. In the present paper the model describing excitations in such a system via the Hubbard Hamiltonian with an electron-phonon interaction is suggested. When taking into account the electron correlations on the ground state only, an integrable system of nonlinear Schrödinger equations with U(1,1) isogroup appears. The composition of the paper is as follows. In Chapter 1 the foundation of the model as well as the getting of the main equations is given. Chapter 2 is devoted to the statement of the Cauchy problem and to the choice of boundary conditions. Chapters 3 and 4 deal with the solution of the Cauchy problem via the Inverse Scattering Method (ISM) under the nonvanishing boundary conditions. Chapter 5 is devoted to the investigation of the interaction between "colored" solitons in the stable medium. In Chapter 6 the solitonic mechanism of the charge transport in the organic salts is presented and the existence of the structural phase transition through the power constant is discussed as well.

1. THE MODEL AND THE MAIN EQUATIONS

The Hamiltonian of the system under consideration[4] is:

$$\mathcal{H} = \mathcal{H}_e + \mathcal{H}_L + \mathcal{H}_{int}\,, \tag{1}$$

where

$$\mathcal{H}_e = t\sum_{i\sigma}\left(c^{+A}_{i\sigma}c^{B}_{i+1\sigma} + c^{+B}_{i\sigma}c^{A}_{i+1\sigma} + \text{h.c.}\right) + \sum_{i\sigma} n_{i\sigma}\left(\frac{U}{2}n_{i-\sigma} - \mu\right), \tag{2}$$

$$\mathcal{H}_L = \frac{M}{2}\sum_n \dot{R}^2_n + \frac{\alpha}{2}\sum_n \left(R_{n+1} - R_n\right)^2, \tag{3}$$

$$\mathcal{H}_{int} = I\sum_{i\sigma}\left(u_i - u_{i+1}\right)\left(c^{+B}_{i\sigma}c^{A}_{i+1\sigma} + c^{+A}_{i\sigma}c^{B}_{i+1\sigma} + \text{h.c.}\right). \tag{4}$$

Here, $c^{+}_{n\sigma}(c_{n\sigma})$ is the creation (annihilation) operator of an electron with spin σ in a Wannier state of the n-th atom, t is the transition amplitude between nearest neighbours, U is the repulsive interaction between electrons of the same atom, μ denotes the chemical potential, M is the mass of an atom in the chain, α denotes the power constant, $R_j = R_{j0} + u_j$ is the position of the j-th atom, u_j is the deviation from the equilibrium position R_{j0}, I denotes the power of the electron-phonon interaction, $n_{i\sigma} = c^{+}_{i\sigma} c_{i\sigma}$ is the number operator, A and B denote proper molecules of the homogeneous dimerized chain[5].

The Heisenberg equations of motion for $c^{A}_{n\sigma}(t)$ give:

$$i\frac{dc^{A}_{i\sigma}}{dt} = [c^{A}_{i\sigma}, H] = Uc^{A}_{i\sigma} n^{A}_{i-\sigma} - \mu c^{A}_{i\sigma} + [t + I(u_i - u_{i+1})]\, c^{B}_{i+1\sigma} + [t + I(u_{i-1} - u_i)]\, c^{B}_{i-1\sigma}. \tag{5}$$

In the quasiclassical approximation[6] we subtract from the operator $c_{i\sigma}$ a small operator addition $\alpha_{i\sigma}$:

$$c_{i\sigma} = \phi_{i\sigma} + \alpha_{i\sigma}, \quad \|\alpha_{i\sigma}\| \ll \phi_{i\sigma}, \tag{6}$$

where $\phi_{i\sigma}$ is a c-number (not Grassman) state function*. The Hamilton equations of motion for $\phi_{i\sigma}(t)$ are:

$$i\dot{\phi}^{A,B}_{j\sigma} = U\phi^{A,B}_{j\sigma} |\phi^{A,B}_{j-\sigma}|^2 - \mu\phi^{A,B}_{j\sigma} + [t + I(u_j - u_{j+1})]\,\phi^{B,A}_{j+1\sigma} + [t + I(u_{j-1} - u_j)]\,\phi^{B,A}_{j-1\sigma}. \tag{7}$$

It is necessary to complete these equations by the lattice oscillations[4]:

$$M\ddot{R}_j = \alpha(R_{j+1} - 2R_j + R_{j-1}) + I\sum_\sigma [\phi^{*A}_{j+1\sigma}(\phi^{B}_{j+1\sigma} - \phi^{B}_{j-1\sigma}) + \phi^{*B}_{j\sigma}(\phi^{A}_{j+1\sigma} - \phi^{A}_{j-1\sigma}) + \text{c.c.}]. \tag{8}$$

To understand the possible mechanism of the charge transfer in the system (1) let us consider a long-wave continuous approximation when $a \to 0$[4]:

$$\frac{u_j}{a} = \frac{R_j}{a} - \frac{R_{j0}}{a} \to u(x,t) - x,$$

*It is interesting to note that for an integrable Fermi system the quasiclassical spectrum coincides with the exact one[7] as in the Bose systems[8].

$$\phi_{j\sigma}(t) \to \phi_\sigma(x,t),$$

$$R_{j\pm1}/a \to u(x,t) \pm u_x(x,t) + \frac{1}{2}u_{xx}(x,t) + \dots, \tag{9}$$

$$\phi_{j\pm1\sigma} \to \phi^\sigma(x,t) \pm \phi^\sigma_x(x,t) + \frac{1}{2}\phi^\sigma_{xx}(x,t) + \dots .$$

In such a way the equations of motion (7) and (8) become:

$$i\phi^{A,B}_{\sigma t} = U\phi^{A,B}_{\sigma} |\phi^{A,B}_{-\sigma}|^2 - \mu\phi^{A,B}_{\sigma} + 2[t + Ia(1 - u_x)](\phi^{B,A}_{\sigma} + \frac{1}{2}\phi^{B,A}_{\sigma xx}), \tag{7'}$$

$$Mu_{tt} = \alpha u_{xx} + \frac{2I}{a}\sum_\sigma \frac{\partial}{\partial x}(\phi^{*A}_\sigma \phi^{B}_\sigma + \text{c.c.}). \tag{8'}$$

To emphasize the role of the electron-phonon interaction in the mechanism of charge transfer, we neglect the Coulomb repulsion of electrons ($U \ll t$) at the first approximation, taking electron correlations on the level of the ground state*. For the antiferromagnetic ground state this leads to the connection:

$$\phi^{B}_{-\sigma} = \phi^{A}_{\sigma} \equiv \phi_\sigma. \tag{10}$$

In the quasistationary limit[18] the first integral of equation (8') reads:

$$u_x(x,t) - \frac{2I}{\alpha a}\sum_\sigma (\phi^*_\sigma \phi_{-\sigma} + \text{c.c.}) = \text{const}. \tag{11}$$

Due to this approximation equation (7') gives the Hartree-Fock-like system with the self-consistent potential[11]:

$$i\phi_{\sigma t} = T\phi_{-\sigma xx} + [2T - (\frac{2I}{\sqrt{\alpha}})^2 \sum_{\sigma'} (\phi^*_{\sigma'}\phi_{-\sigma'} + \text{c.c.})]\,\phi_{-\sigma} - \mu\phi_\sigma, \tag{12}$$

where $T = t + Ia(1 - \text{const})$, $\sigma = (\uparrow, \downarrow)$.

Introducing the amplitudes of mixtures spin states:

$$c_{\pm}(x,t) = \phi_\uparrow(x,t) \pm \phi_\downarrow(x,t), \tag{13}$$

one obtains the system of two bound nonlinear equations:

*Note by the way that the integrability of the considered nonlinear system admits a more correct consideration of the neglected Coulomb contribution to the transfer mechanism by the multisoliton perturbation theory.

$$ic_{+t} = Tc_{+xx} + [2T - (\frac{2I}{\sqrt{a}})^2(|c_+|^2 - |c_-|^2)]c_+ - \mu c_+$$
$$-ic_{-t} = Tc_{-xx} + [2T - (\frac{2I}{\sqrt{a}})^2(|c_+|^2 - |c_-|^2)]c_- + \mu c_- . \tag{14}$$

Some special single-soliton solutions of the system (14) have been discussed in papers [4,9,17]. By the gauge-scaling transform:

$$c_\pm(x, t) \to \tilde{c}_\pm(x, t) = c_\pm(\sqrt{T}x, t)e^{i\mu t} \tag{15}$$

and going to the new variables:

$$\psi(x, t) = \begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}(x, t) = \begin{pmatrix}\tilde{c}^*_+\\ \tilde{c}_-\end{pmatrix}(x, t) \tag{16}$$

the system (14) takes the canonical form of the U(1,1) NLSE model[9]:

$$i\psi_{1t} + \psi_{1xx} + \kappa(|\psi_1|^2 - |\psi_2|^2 - \rho^2)\psi_1 = 0,$$
$$i\psi_{2t} + \psi_{2xx} + \kappa(|\psi_1|^2 - |\psi_2|^2 - \rho^2)\psi_2 = 0, \tag{17}$$

where $\kappa = (2I/\sqrt{a})^2$, $\rho^2 = -2/\kappa$.

In what follows we shall study the above system via the Inverse Scattering Method (ISM) in detail.

2. THE CAUCHY PROBLEM AND THE CHOICE OF THE BOUNDARY CONDITIONS

As is well-known[10] the ISM allows one to set and investigate in detail the Cauchy problem under the proper boundary conditions. Because of the main interest to the dynamics of the phase transition from the antiferromagnetic ground state, it is natural to consider the nonvanishing, (constant) at both infinities, boundary conditions:

$$q(x, t) \to q_\pm \tag{18}$$
$$x \to \pm\infty .$$
$$q_x(x, t) \to 0 \tag{19}$$

Here, more convenient variables are introduced:

$$q(x, t) = \begin{pmatrix}q_1\\ q_2\end{pmatrix}(x, t) = \sqrt{\frac{2}{\kappa}}\,\psi(x, t), \tag{20}$$

for which the matrix realization of (17) reads:

$$iq_t + q_{xx} + 2((\bar{q}q) - \rho^2)q = 0, \tag{21}$$

where $(\bar{q}q) \equiv |q_1|^2 - |q_2|^2$, $\bar{q} = q^+\gamma_0$, $\gamma_0 = \mathrm{diag}(1,-1)$.

It is easy to check that from (21) by virtue of (18) and (19) it follows that a correct setting of the problem implies:

$$(\bar{q}_+q_+) = (\bar{q}_-q_-) = \rho^2. \tag{22}$$

The possibility of the complete study of the system (21) comes from the corresponding linear problem:

$$\phi_x = U\phi, \tag{23}$$

$$\phi_t = V\phi, \tag{24}$$

where

$$U(x, \lambda) = -i\lambda\Sigma + Q(x),$$

$$V(x, \lambda) = \left(\begin{array}{c|c} 4i\lambda^2 - i(\bar{q}q - \rho^2) & 2i\lambda\bar{q} - \bar{q}_x \\ \hline 2i\lambda q + q_x & i(q\otimes\bar{q}) - i\rho^2 I_2 \end{array}\right),$$

$$\Sigma = \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & -I_2 \end{array}\right), \quad Q(x) = \left(\begin{array}{c|c} 0 & -i\bar{q}(x) \\ \hline -iq(x) & 0\cdot I_2 \end{array}\right), \quad I_2 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}.$$

The integrability condition for the system (23)-(24) generates the nonlinear model (21)-(18)-(19).

3. THE DIRECT PROBLEM

Let us consider the spectrum problem (23) on the axis $-\infty < x < \infty$. Introduce the matrix Jost solutions $\Phi_\pm(x, \lambda)$ which are determined by their asymptotic behaviour:

$$\Phi_\pm(x, \lambda) \xrightarrow[x \to \pm\infty]{} X_\pm(x, \lambda), \tag{25}$$

where

$$X_\pm(x, \lambda) = \chi_\pm(\lambda)e^{i\Lambda x}, \quad \Lambda = \mathrm{diag}(-\zeta, \zeta, \lambda),$$

$$\chi_\pm(\lambda) = \begin{pmatrix} \lambda+\zeta & \lambda-\zeta & 0 \\ q_{\pm1} & q_{\pm1} & q^*_{\pm2} \\ q_{\pm2} & q_{\pm2} & q^*_{\pm1} \end{pmatrix}, \quad \zeta^2 = \lambda^2 + \rho^2, \tag{26}$$

$$\det\Phi_\pm(x, \lambda) = \det X_\pm(x, \lambda) = 2\zeta\rho^2 e^{i\lambda x} .$$

Since the Jost solutions form the Fundamental system of solutions, Φ_+ is a linear combination of Φ_-:

$$\Phi_-(x,\lambda) = \Phi_+(x,\lambda)\, S(\lambda), \tag{27}$$

where $S(\lambda)$ is the scattering matrix for problem (23). Let us examine the symmetry properties of the Jost solutions. Consider for that the conjugate to (23) equation:

$$\Phi^+(x,\lambda)\,(-i\,\Sigma\,\partial_x + Q^+(x)) = \lambda^*\,\Phi^+(x,\lambda).$$

Due to the non-Hermitean character of the linear problem (23) its spectrum in general is complex.

Having used the fact that in our case: $\Gamma Q^+ \Gamma = -Q$, $\Gamma = \mathrm{diag}(1,1,-1)$, and hence $\partial/\partial x\,(\Gamma\Phi^+(x,\lambda)\,\Gamma\,\Phi(x,\lambda)) = 0$, for real λ and $\zeta(\lambda)$ we have: $\Gamma\Phi^+(x,\lambda)\,\Gamma\,\Phi(x,\lambda) = A$. By the appropriate choice of the Jost solutions [15] the last equation becomes:

$$\bar{\Phi}(x,\lambda)\,\Phi(x,\lambda) = I, \qquad \bar{\Phi} \equiv \Gamma\Phi^+\Gamma. \tag{28}$$

It means by the way that for real λ and $\zeta(\lambda)$ the Jost solutions $\Phi_\pm$ belong to SU(2,1) group. From (26) and (28) we have the unimodularity condition:

$$\det S(\lambda) = 1 \tag{29}$$

and the pseudounitariry one:

$$\bar{S}(\lambda)\,S(\lambda) = I, \qquad \bar{S} \equiv \Gamma S^+ \Gamma. \tag{30}$$

Besides, from (27) and (28) it follows that:

$$S_{ik}(\lambda) = \bar{\Phi}_{+i}(x,\lambda)\,\Phi_{-k}(x,\lambda). \tag{31}$$

We have so far considered the properties of the S-matrix and Jost solutions for real λ and $\zeta(\lambda)$. Let us define their analytic behaviour in the λ-plane. Note that the function $\zeta(\lambda) = \sqrt{\lambda^2 + \rho^2}$ $(\rho^2 < 0)$ is defined on the two-fold Riemanian surface whose first sheet is glued with the second one along cuts $(-\infty, -\rho)$ and $(\rho, +\infty)$. The analytical properties of the Jost functions can be derived from the following integral equations:

$$\Phi_\pm(x,\lambda) = X_\pm(x,\lambda) + \int_x^{\pm\infty} dy\, X_\pm(x,\lambda)\, X_\pm^{-1}(y,\lambda)\,(Q_\pm - Q(y))\,\Phi_\pm(y,\lambda) \tag{32}$$

which are equivalent to equations (23) under the boundary conditions (18) and (19). Supposing that the potential $Q(x)$ tends to its asymptotics $Q_\pm$ fast enough, one can then ensure that the Jost solutions Φ_{+2} and Φ_{-1} can be analytically continued on the upper sheet of the Riemanian surface $(\mathrm{Im}\,\zeta > 0)$, solutions

Φ_{+1} and Φ_{-2} are analytical functions of λ on the lower sheet $(\mathrm{Im}\,\zeta < 0)$, and the solutions $\Phi_{\pm 3}$ are defined on the real axis $(\mathrm{Im}\,\lambda = 0)$ only and have no analytical continuation. From (31) it follows that the function $s_{11}(\lambda, \zeta)$ is analytical on the upper sheet $(\mathrm{Im}\,\zeta > 0)$.

The spectrum of the problem is more complicated than in the case of U(0,2) NLSE [15] but has the same peculiarities.

The discrete spectrum lies in the gap $(-\rho, \rho)$ between cuts and is defined by zeroes of the function $s_{11}(\lambda, \zeta)$. In the general case of non Hermitean operator U there are no limitations on the number, location and multiplicity of the zeroes of $s_{11}(\lambda, \zeta)$.

The continuous spectrum consists of two parts. The first lies on both the cuts of the Riemannian surface apart from the gap $(-\rho, \rho)$. The second one may appear on the real axis of the λ-plane, leading to interference with the zeroes of the gap and generating the peculiar soliton-like solution [11,12]. At the points of the discrete spectrum we have:

$$\Phi_{-1}(x,\lambda_n) = c_{2n}\,\Phi_{+2}(x,\lambda_n) + c_{3n}\,\Phi_{+3}(x,\lambda_n) \tag{33}$$

with $s_{11}(\lambda_n, \zeta_n) = 0$, $c_{2n} = s_{21}(\lambda_n, \zeta_n)$, $c_{3n} = s_{31}(\lambda_n, \zeta_n)$.

So, the independent set of the scattering data for the problem (23) is:

$$\{r_{21}(\lambda),\ r_{31}(\lambda),\ c_{2n},\ c_{3n},\ \lambda_n,\ n = 1,2,\ldots,N\}, \tag{34}$$

with $r_{21} = s_{21}/s_{11}$, $r_{31} = s_{31}/s_{11}$.

Now let us obtain the time evolution of the spectral data. Using the results of paper [13], one gets:

$$iS_t(\lambda, t) = [\Pi(\lambda), S(\lambda, t)], \tag{35}$$

where $\Pi(\lambda) = \mathrm{diag}\,((\lambda+\zeta)^2, (\lambda-\zeta)^2, 0)$.

Due to the fact that eigenvalues λ_n as zeroes of s_{11} are independent of time there is an infinite series of the local conservation laws.

The first three of these are [13]:

$$\begin{aligned} I_1 &= \int_{-\infty}^{\infty} dx\,(\bar{q}q - \rho^2)(x,t), \\ I_2 &= \int_{-\infty}^{\infty} dx\,(\bar{q}q_x)(x,t), \\ I_3 &= \int_{-\infty}^{\infty} dx\,(\bar{q}q_{xx} + (\bar{q}q)^2 - \rho^2)(x,t). \end{aligned} \tag{36}$$

Note, that the first two integrals are the particle number and momentum of the system, respectively. And its energy is the following linear combination of I_3 and I_1:

$$H = I_3 - 2\rho^2 I_1. \tag{37}$$

So, the condensate density ρ^2 plays the role of a "chemical potential" in the many-particle system under consideration.

4. THE INVERSE PROBLEM

Here we consider the problem of the potential reconstruction with respect to the known scattering data (34) evolving according to (35). From (32) one can derive the triangular representation for the Jost solution Φ_+:

$$\Phi_+(x, \lambda) = X_+(x, \lambda) - \int_x^\infty ds\, K(x, s)\, X_+(s, \lambda). \tag{38}$$

Inserting (38) into the linear problem (23), we get the differential equation on kernel $K(x, y)$:

$$\Sigma K_x(x, y) + K_y(x, y)\Sigma = i\tilde{Q}(x) K(x, y) - iK(x, y)\tilde{Q}_+ \tag{39}$$

with the boundary conditions:

$$\begin{cases} [K(x, x), \Sigma] = i(\tilde{Q}_+ - \tilde{Q}(x)) \\ K(x, y) \to 0, \quad y \to \infty, \qquad \text{where} \end{cases} \tag{40}$$

$$\tilde{Q}(x) = \begin{pmatrix} 0 & -q_1^*(x) & q_2^*(x) \\ q_1(x) & 0 & 0 \\ q_2(x) & 0 & 0 \end{pmatrix}, \qquad \tilde{Q}_\pm = \lim_{x \to \pm\infty} \tilde{Q}(x).$$

One may then express the potential $q(x)$ through the elements of the kernel: $K(x, x)$:

$$\begin{cases} q_1(x) = q_{+1} + 2i\, K_{21}(x, x) \\ q_2(x) = q_{+2} + 2i\, K_{31}(x, x). \end{cases} \tag{41}$$

In addition: $K^*_{12}(x, x) = -K_{21}(x, x)$, $K^*_{13}(x, x) = K_{31}(x, x)$.

To get the Marchenko equation following Zakharov and Shabat [14] let us integrate the relation:

$$\frac{1}{2\pi\zeta}\left(\frac{1}{s_{11}(\lambda)}\Phi_{-1}(x, \lambda) - X_{+1}(x,\lambda)\right)e^{i\zeta y} = \frac{1}{2\pi\zeta}(\Phi_{+1}(x, \lambda) -$$

$$- X_{+1}(x, \lambda) + r_{21}(\lambda)\,\Phi_{+2}(x, \lambda) + r_{31}(\lambda)\,\Phi_{+3}(x, \lambda))e^{i\zeta y}.$$

along the infinite circle at the complex λ-plane on the upper sheet of the Riemanian surface ($\operatorname{Im}\zeta > 0$). One can apply the residue techniques at points λ_n to the left hand-side of this relation (under condition $y > x$).

The result is as follows:

$$i\sum_n \frac{\Phi_{-1}(x, \lambda_n)}{\zeta_n s'_{11}(\lambda_n, \zeta_n)} e^{i\zeta_n y} = i\sum_n \frac{c_{2n}\Phi_{+2}(x, \lambda_n) + c_{3n}\Phi_{+3}(x, \lambda_n)}{\zeta_n s'_{11}(\lambda_n, \zeta_n)} e^{i\zeta_n y} \equiv$$

$$\equiv \sum_n (\mu_n^{(1)}\Phi_{+2}(x, \lambda_n) + \mu_n^{(2)}\Phi_{+3}(x, \lambda_n))e^{i\zeta_n y}.$$

The right hand-side can be represented in the form (supposing the existence of the corresponding limits for $\Phi_{\pm 3}$ and r_{31} at least near the Bargmann strip):

$$-K(x, y)\begin{pmatrix} 0 \\ q_{+1} \\ q_{+2} \end{pmatrix} + \begin{pmatrix} F_1^{(1)}(x + y) + iF_2^{(1)\prime}(x + y) \\ q_{+1}F_2^{(1)}(x + y) \\ q_{+2}F_2^{(1)}(x + y) \end{pmatrix} + F_3^{(1)}(x, y)\begin{pmatrix} 0 \\ q^*_{+2} \\ q^*_{+1} \end{pmatrix} -$$

$$- \int_x^\infty ds\, K(x, s)\left[\begin{pmatrix} F_1^{(1)}(s + y) + iF_2^{(1)\prime}(s + y) \\ q_{+1}F_2^{(1)}(s + y) \\ q_{+2}F_2^{(1)}(s + y) \end{pmatrix} + F_3^{(1)}(s, y)\begin{pmatrix} 0 \\ q^*_{+2} \\ q^*_{+1} \end{pmatrix}\right],$$

where

$$F_1^{(1)}(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\xi\, b_1(\xi) e^{i\xi z},$$

$$F_2^{(1)}(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\xi\, b_2(\xi) e^{i\xi z},$$

$$F_3^{(1)}(x, y) = \frac{1}{2\pi}\int \frac{d\lambda}{\xi}\, r_{31}(\lambda, \xi)\, e^{i(\lambda x + \xi y)},$$

$$b_1(\xi) = \frac{1}{2}[r_{21}(\lambda, \xi) + r_{21}(-\lambda, \xi)],$$

$$b_2(\xi) = \frac{1}{2\lambda}[r_{21}(\lambda, \xi) - r_{21}(-\lambda, \xi)], \quad \xi = \operatorname{Re}\zeta.$$

Finally, the Marchenko equations become:

$$K(x,y)\begin{pmatrix}0\\ q_{+1}\\ q_{+2}\end{pmatrix}+\begin{pmatrix}F_1(x+y)+iF_2'(x+y)\\ q_{+1}F_2(x+y)\\ q_{+2}F_2(x+y)\end{pmatrix}+F_3(x,y)\begin{pmatrix}0\\ q^*_{+2}\\ q^*_{+1}\end{pmatrix}-$$
$$-\int_x^\infty ds\, K(x,s)\left[\begin{pmatrix}F_1(s+y)+iF_2'(s+y)\\ q_{+1}F_2(s+y)\\ q_{+2}F_2(s+y)\end{pmatrix}+F_3(s,y)\begin{pmatrix}0\\ q^*_{+2}\\ q^*_{+1}\end{pmatrix}\right]=0, \tag{42}$$

where

$$F_1^{(2)}(z)=-\sum_n \mu_n^{(1)}\lambda_n e^{i\zeta_n z},$$
$$F_2^{(2)}(z)=-\sum_n \mu_n^{(1)} e^{i\zeta_n z},$$
$$F_3^{(2)}(x,y)=-\sum_n \mu_n^{(2)} e^{i(\lambda_n x+\zeta_n y)},$$
$$F_\alpha=F_\alpha^{(1)}+F_\alpha^{(2)},\quad \alpha=1,2,3.$$

When deriving the equations (42) the interference between discrete and continuous spectra (mentioned above) is neglected. Phenomena due to the overlap as well as their most probable generation mechanism will be discussed below.

In the case of reflectionless potentials the Marchenko equations reduce to the system of $2N$ (where N is the number of zeroes λ_n) linear algebraic equations, which admit the exact solution. So, we look for a solution of (42) in the form:

$$K(x,y)=\sum_{n=1}^{N} K_n(x)\,Y_n(y,\lambda_n), \tag{43}$$

where $K_n(x)$ is the column vector, and $Y(y,\lambda_n)=e^{i\zeta_n y}(a,b,c)$ is the row vector. In particular, the single-soliton kernel $(N=1)$ assumes the form:

$$K_{21}(x,x)=\frac{a e^{i\zeta x}(q_{+1}\mu_1 e^{i\zeta x}+q^*_{+2}\mu_2 e^{i\lambda x})}{d-[a(\lambda-\zeta)+bq_{+1}+cq_{+2}]\frac{\mu_1}{2i\zeta}e^{2i\zeta x}-(bq^*_{+2}+cq^*_{+1})\frac{\mu_2}{i(\lambda+\zeta)}e^{i(\lambda+\zeta)x}},$$
$$K_{31}(x,x)=K_{21}(x,x)\big|_{q_{+1}\to q_{+2}};\quad d=bq_{+1}+cq_{+2}. \tag{44}$$

Here $\zeta_1=\zeta$, $\lambda_1=\lambda$, $\mu_1^{(1)}=\mu_1$, $\mu_1^{(2)}=\mu_2$. Since it is difficult to analyze this solution in general, we consider its special

reductions. The most interesting solutions, appearing when

$$a=-(\lambda+\zeta),\quad b=q^*_{+1},\quad c=-q^*_{+2},\quad d=\rho^2,$$

are:

$$\begin{cases} q_1(x,t)=q_{+1}\dfrac{e^{i\alpha}+\dfrac{\zeta}{i\mu_1}e^{-2i\zeta x}}{1+\dfrac{\zeta}{i\mu_1}e^{-2i\zeta x}}+\dfrac{2\zeta}{\lambda-\zeta}q^*_{+2}\dfrac{\dfrac{\mu_2}{\mu_1}e^{i(\lambda-\zeta)x}}{1+\dfrac{\zeta}{i\mu_1}e^{-2i\zeta x}} \\ q_2(x,t)=q_1(x,t)\big|_{q_{+1}\to q_{+2}}, \end{cases} \tag{45}$$

where $e^{i\alpha}=\frac{\lambda+\zeta}{\lambda-\zeta}$ is the condensate phase, and

$$\begin{cases}\mu_1(t)=\mu_1(0)\,e^{-4i\lambda\zeta t}\\ \mu_2(t)=\mu_2(0)\,e^{-i(\lambda+\zeta)^2 t}.\end{cases}$$

We note that the solution (45) is a complexificated version of the "drop-bubble" solution /19/. But the real reduction of solution (45) ($\mathrm{Im}\,\lambda=0$) leads to another well-known "double-bubble" solution /19/:

$$q(x,t)=\frac{q_+}{\lambda-i\nu}(\lambda-i\nu\,\mathrm{th}\,\nu z),\qquad \text{where} \tag{46}$$
$$q^T=(q_1,q_2),\quad z=x-2\lambda t-x_0,\quad e^{2\nu x_0}=\frac{\mu_1(0)}{\nu},$$
$$\zeta=i\nu,\quad \rho^2=-(\lambda^2+\nu^2).$$

It is quite easy to explain this fact if one remembers that under the Hermitean reduction there takes place the interference between the second branch of the continuous spectrum (a weak background) and zeroes of the discrete spectrum from the gap (kink). As a result of this "interaction", a peculiar (in the framework of the ISM) soliton-like solution ("bubble-drop") appears. Surely, to obtain such a specific soliton generation via the ISM it is necessary to take into account (when getting the Marchenko equations) the existence of a spare continuous branch. In fact, this leads to the "renormalization" of the kink solution (46) on the constant factor and to the generation (due to the plane-wave "tail" $e^{i\lambda x}$) of a new "drop"-like solution /19/.

Finally, quite a stable bion-like configuration is generated:

$$q(x,t)=\sqrt{\frac{\beta}{2}}\left[\frac{q_+}{\lambda-i\nu}(\lambda-i\nu\,\mathrm{th}\,\nu z)+\frac{i\nu}{\lambda-i\nu}\sigma_1 q^*_+ e^{i\theta}\,\mathrm{sech}\,\nu z\right], \tag{47}$$

where $\theta = \lambda x - (\lambda^2 - \nu^2)t - i\phi$, $\quad e^{\phi} = \frac{\mu_2(0)}{\nu}\sqrt{\frac{\nu}{\mu_1(0)}} = \sqrt{\frac{2}{\beta} - 1}$.

β is the "switch" parameter.

When $\beta_c = 2$ the interference between background and kink disappears.

Note that the parameter β may be connected with the power constant κ leading to interesting consequences [12].

Concluding the section it is important to underline that a weakly distorted ($|r_{21}| \ll 1$, $|r_{31}| \ll 1$) "double-bubble" (46) asymptotically (when $t \to \pm\infty$) tends to the pure soliton solution as $1/t$ [16]. As is pointed out in paper [15] this fact is due to the "medium" of a finite density ρ^2, which accelerates the releaze process of perturbed soliton from a weak continuous background.

5. THE SOLITON INTERACTION

Let us consider the traditional application of the ISM, namely the soliton scattering. First of all consider the collision of two "colored" kinks moving with velocities $2\lambda_1$ and $2\lambda_2$, respectively, so that $\lambda_1 > \lambda_2$ (i.e., the possibility of bound solitons is excluded). To study the two-soliton interaction it is sufficient to consider the asymptotical behaviour of the two-soliton solution. That is:

$$q^{II}(x,t) = q_+ + 2iq_+ \frac{\frac{2}{\nu_1+\nu_2}[\lambda_1+\lambda_2+i(\nu_1+\nu_2)] - (\lambda_1+i\nu_1)\left(\frac{1}{\nu_2}+\frac{e^{2\nu_2 x}}{\mu_{12}}\right) - (\lambda_2+i\nu_2)\left(\frac{1}{\nu_1}+\frac{e^{2\nu_1 x}}{\mu_{11}}\right)}{\rho^2\left(\frac{1}{\nu_1}+\frac{e^{2\nu_1 x}}{\mu_{11}}\right)\left(\frac{1}{\nu_2}+\frac{e^{2\nu_2 x}}{\mu_{12}}\right) - \frac{2}{(\nu_1+\nu_2)^2}(\rho^2 - \lambda_1\lambda_2 - \nu_1\nu_2)}$$

where $q^T = (q_1, q_2)$.

When $t \to \pm\infty$ the solution in fact decays into separate kinks:

$$q^{II}(x,t) \underset{t\to+\infty}{\to} q^{I}(x - 2\lambda_1 t, x_1^+, q_+, a_1^+) + q^{I}(x - 2\lambda_2 t, x_2^+, q_+, a_2^+),$$

$$q^{II}(x,t) \underset{t\to-\infty}{\to} q^{I}(x - 2\lambda_1 t, x_1^-, q'_+, a_1^-) + q^{I}(x - 2\lambda_2 t, x_2^-, q'_+, a_2^-).$$

As a result of the elastic two-kink scattering we have the following effects.

A. The Center-of-Mass Translations

The first kink (having higher rate) admits the positive shift:

$$\delta x_1 = x_1^+ - x_1^- = \frac{1}{2\nu_1}\ln\frac{(\nu_1+\nu_2)^2(\lambda_1^2+\nu_1^2)}{(\nu_1\lambda_2-\nu_2\lambda_1)^2} \tag{48a}$$

and the second, respectively, the negative one by the amount:

$$\delta x_2 = x_2^+ - x_2^- = -\frac{1}{2\nu_2}\ln\frac{(\nu_1+\nu_2)^2(\lambda_2^2+\nu_2^2)}{(\nu_1\lambda_2-\nu_2\lambda_1)^2}. \tag{48b}$$

Due to: $\rho^2 = -(\lambda_1^2+\nu_1^2) = -(\lambda_2^2+\nu_2^2)$ from (48a,b) there follows the conservation law of the soliton center-of-mass:

$$\nu_1\delta x_1 + \nu_2\delta x_2 = 0. \tag{49}$$

Note that in the limit q_{+1} (or q_{+2}) $\to 0$ and when $\lambda_1 = 0$ the relations (48a,b) render the Zakharov-Shabat results [14].

B. "Color" Change

Like in the case of U(2,0) NLSE solitons studied by Manakov [16] we also may say about the "polarization" (or "color") of the solution (46). Nevertheless, the nature of this degree of freedom is quite different in both cases. In Manakov's case it is determined by the coefficients c_{21} and c_{31} of the Jost solutions (33). In the case of "colored" kinks (46) its appearance is due to the presence of the condensate, i.e., it is influenced by the nonvanishing boundary conditions ($q_\pm \neq 0$). This leads to the specific "color" change via the U(1) transform:

$$q_+ \to q'_+ = q_+ e^{i\alpha_2} \tag{50a}$$

for the first kink, and similarly as:

$$q_+ \to q'_+ = q_+ e^{i\alpha_1} \tag{50b}$$

for the second one. Here $e^{i\alpha_n} = \frac{\lambda_n + i\nu_n}{\lambda_n - i\nu_n}$, $n = 1, 2$ is the proper one-kink condensate phase.

We note that in contrast with the Manakov case [16] the effects of "color" exchange are absent. This is due to the vanishing of the coefficient s_{13} when **Hermitian** reduction (46) is performed.

C. Phase Changes

As a result of elastic soliton scattering the kink phases are changed as well:

$$\delta a_1 = a_1^+ - a_1^- = a_1^- - \left(-a_2 - i\ln\left(1 + \frac{2i}{\rho^2}\frac{\Delta_2}{\Delta_1}\right)\right) \tag{51a}$$

$$\delta\alpha_2 = \alpha_2^+ - \alpha_2^- = \alpha_2 - \left(-\alpha_1 - i\ln\left(1 + \frac{2i}{\rho^2}\frac{\Delta_2}{\Delta_1}\right)\right), \tag{51b}$$

i.e.,

$$\delta\alpha_1 = \alpha + i\ln\left(1 + \frac{2i}{\rho^2}\frac{\Delta_2}{\Delta_1}\right) = \delta\alpha_2, \tag{52}$$

where $\Delta_1 = -\dfrac{(\nu_1\lambda_2 - \nu_2\lambda_1)^2}{\rho^2(\nu_1 + \nu_2)^2}$, $\Delta_2 = \dfrac{\nu_2 - \nu_1}{\nu_2 + \nu_1}[\nu_1(\lambda_1 + i\nu_1) - \nu_2(\lambda_2 + i\nu_2)]$.

Here, $\alpha = \alpha_1 + \alpha_2$ is the two-kink condensate phase. In particular, it follows from (52) that $\delta\alpha$ is proportional to α.

One should expect that the interaction picture mentioned above becomes more complicated when bion-like solitons (47) take part in the collision. Indeed, analyzing the two-bion solution, one may show that in addition to the effects (A,B,C), we obtain the "renormalization" of the "drop" amplitudes:

$$\delta\phi_1 = \phi_1^+ - \phi_1^- = \ln\frac{\Delta_2}{(\lambda_1 + i\nu_1)(\nu_1 - \nu_2)\sqrt{\Delta_1}}, \tag{53a}$$

$$\delta\phi_2 = \phi_2^+ - \phi_2^- = \ln\frac{\Delta_2}{(\lambda_2 + i\nu_2)(\nu_1 - \nu_2)\sqrt{\Delta_1}}. \tag{53b}$$

We note that due to (47) there follows from (53) the "renormalization" of the parameter β as well

6. DISCUSSION

Let us come back to the initial problem and discuss the results obtained above on the language of electron amplitudes. Since the analysis of the "controlled" soliton (47) is rather complicated and requires a special treatment, we concentrate our attention on the kink solution (46) only. Performing step by step the transforms (20), (16), (15) and (13) for spin up and down state amplitudes one gets:

$$\begin{aligned} \phi_\uparrow(x,t) &= \sqrt{\frac{\kappa}{8}}\, e^{-i\mu t}(q_1(x,t) + q_2^*(x,t)), \\ \phi_\downarrow(x,t) &= \sqrt{\frac{\kappa}{8}}\, e^{-i\mu t}(q_1(x,t) - q_2^*(x,t)). \end{aligned} \tag{54}$$

Using the explicit form of solution (46), we have:

$$\begin{aligned} |\phi_\uparrow|^2 &= \frac{\kappa}{8}(\lambda^2 + \nu^2 \mathrm{th}^2\,\nu z)(|q_{+1}|^2 + |q_{+2}|^2 + 2|q_{+1}|\,|q_{+2}|\cos\Omega) \\ |\phi_\downarrow|^2 &= \frac{\kappa}{8}(\lambda^2 + \nu^2 \mathrm{th}^2\,\nu z)(|q_{+1}|^2 + |q_{+2}|^2 - 2|q_{+1}|\,|q_{+2}|\cos\Omega), \end{aligned} \tag{55}$$

with $\Omega = \arg q_{+1} - \arg q_{+2}$.

So, the time evolution of the average occupation number $n(x,t)$ from the initial state n_+ is

$$n(x,t) = |\phi_\uparrow|^2 + |\phi_\downarrow|^2 = \frac{n_+}{\lambda^2 + \nu^2}(\lambda^2 + \nu^2 \mathrm{th}^2\,\nu z), \tag{56}$$

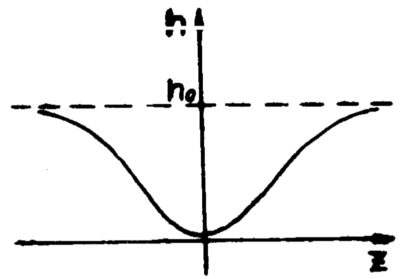
where $n_\pm = \lim\limits_{x\to\pm\infty} n(x,t)$. Besides: $n_+ = n_- = n_0 = \frac{\kappa}{4}(|q_{+1}|^2 + |q_{+2}|^2)$.

Similarly, for the time evolution of the average spin density (magnetization) we have:

$$m(x,t) = |\phi_\uparrow|^2 - |\phi_\downarrow|^2 = \frac{m_+}{\lambda^2 + \nu^2}(\lambda^2 + \nu^2 \mathrm{th}^2\,\nu z), \tag{57}$$

where $m_\pm = \lim\limits_{x\to\pm\infty} m(x,t)$, $m_+ = m_- = m_0 = \frac{\kappa}{2}|q_{+1}|\,|q_{+2}|\cos\Omega$.

We note that $n(x,t)$ is the localized charge density wave (CDW). It plays an important role in the nonlinear mechanism of the charge transfer for the model of organic salts under consideration. The figure displays the density $n(x,t)$ as a function of $z = x + 2\lambda t$ for a soliton moving with the velocity $v = -2\lambda$. The specific dependence of the soliton amplitude on its velocity is due to the hole-like behaviour of the considered solution. To that the soliton velocity has an upper boundary $v^2 = 4\lambda^2 \le 4\rho^2$, and the maximum soliton amplitude is n_0.



Using the quasiclassical approximation one may calculate the soliton distribution functions through their amplitudes and velocities. In addition to charge transport in our system there is a "spin transport" via the localized spin density wave (SDW) $m(x,t)$. It has a form similar to the CDW one. Note that maximum density of "spin transport" takes place when $\arg q_{+1} = \arg q_{+2}$. In the case when $\arg q_{+1} - \arg q_{+2} = \frac{\pi}{2}$ the charge transport is via the spinless kink.

In conclusion we note that the integrable model of the U(1,1) NLSE considered above may be the simplest exactly solvable model that permits the structural phase transition. This unique property is due to the noncompactness of the symmetry group U(1,1). The noncompactness leads to the co-existence in the framework of the model of three different phases. They are:

(1) "double-drop" $(U(1,0) \otimes U(1,0))$
(2) "double-bubble" $(U(0,1) \otimes U(0,1))$
(3) "drop-bubble" $(U(1,0) \otimes U(0,1))$

The most 'intriguing is the existence of the heterophase state ("drop-bubble"). From this point of view the analysis performed above of the U(1,1) NLSE model via the ISM may be easily translated onto the time dynamics of the homophase and heterophase structural transitions in organic compounds (salts) with charge transfer, in the system of weakly non-ideal gas mixtures, in quasi-one-dimensional systems like conductor-semiconductor-insulator and so on. For this reason it is very interesting to construct and investigate in detail via such a model the temperature dynamics of these phase transitions.

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Федянин В.К. и др. E17-83-755

Взаимодействие солитонов в модели органической соли с переносом заряда

Предложена интегрируемая модель для описания нелинейного механизма переноса заряда в органических соединениях типа соли TTF-TCNQ на основе двухподрешеточной модели Хаббарда с учетом электрон-фононного взаимодействия. Показано, что в рассматриваемой модели наряду с обычными бесспиновыми заряженными солитонами существуют солитоны, переносящие как заряд, так и спин. Методом обратной задачи рассеяния исследована динамика взаимодействия "цветных" солитонов в устойчивой среде. Обсуждается возможность структурного фазового перехода по константе связи.

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Fedyanin V.K. et al. E17-83-755

On Interaction between Solitons in the Model of Organic Charge Transfer Salts

An integrable model based on the two-sublattice Hubbard model with electron-phonon interaction is suggested for the description of the nonlinear transport properties of the quasi-one-dimensional organic compounds like TTF-TCNQ salts. It is shown that besides usual spinless charge solitons the model contains solitons transporting both charge and spin. The interaction dynamics of "colored" solitons in the stable medium is investigated via the Inverse Scattering Method. The existence of structural phase transition through the power constant is discussed.

The investigation has been performed at the Laboratory of Computing Techniques and Automation and the Laboratory of Theoretical Physics, JINR.

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