Fizika Nizkikh Temperatur 1996, V. 22, No 3, p. 322–326

Dynamics of transformation of conduction electrons into charge-density-wave soliton at low temperatures

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Submitted September 11, 1995, revised manuscript received September 25, 1995

The analytical model which describes the dynamics of transformation of conduction electrons into nonlinear charge-carrying excitations of CDW in quasi-one-dimensional Peierls–Frohlich conductors is formulated and studied by the inverse scattering transformation method. The pair of self-trapped conduction electrons transform into a charged 2π-kink localized in a single conducting chain and surrounded by dipoles in neighboring chains

The commonly accepted model for the Peierls–Frohlich quasi-one-dimensional charge-density-wave (CDW) conductors relates their unusual transport properties, i. e. nonlinear conductivity, memory effects, etc, to the phase of the CDW order parameter, $\Delta \exp(i\varphi)$, where the modulus Δ is the Peierls energy gap in a quasiparticle spectrum, and φ governs the dynamics of the CDW condensate (the collective excitations of the occupied valence band). The phase dynamics description has been successful in explaining bulk characteristics (see, e.g., reviews [1–3]). However, one principal aspect of the CDW physics, viz. the problem of interaction of the current-carrying CDW phase deformations with conduction electrons, remains unresolved and still arises controversial explanations.

The basic feature of quasi-one-dimensional CDW conductors such as, e.g., TaS_3 is the instability of conduction electrons against the self-trapping and conversion into the valence band where electrons transform into new collective charge carriers. Self-trapping is connected with local gap deformations in conducting chains. The potential barrier for the self-trapping is $\sim \Delta$, the time interval of the gap deformation is of order of ω^{-1} (ω is the frequency of the Peierls phonons which is of order of the Debye frequency [4-6]), and the interchain interaction is of order T_c (T_c is the temperature of the Peierls transition). In a weakly coupled array of highly conducting chains, $T_c \ll \Delta$, the self-trapping of electrons occurs in individual chains independently, and the charge transformations proceeds in two steps, each characterized by the own time scale t_1 : transfer of conduction electrons into the valence band in a single chain, $t_1 \sim \omega^{-1}$, and formation of a collective charge carrier in this chain, $t_2 \gg t_1$. The time t_2 is the intrinsic scale of the CDW phase Hamiltonian at $\Delta = const$ [3–5].

The collective CDW charge, ρ, and the current, j, densities in a single chain are related to phase gradients via the Frohlich relations

$$\rho = \frac{e}{\pi}\frac{\partial\varphi}{\partial x}, \quad j = -\frac{e}{\pi}\frac{\partial\varphi}{\partial t}. \tag{1}$$

When q electrons are converted into the CDW condensate, the phase acquires a local deformation with the net phase shift

$$\delta\varphi = \varphi(x=\infty) - \varphi(x=-\infty) = q\pi . \tag{2}$$

The final stage of conversion is aggregation of individual phase deformations in different chains to a three-dimensional array, $t \sim t_3 \gg t_2$. The time t_3 can be attributed to a long-range Coulomb interaction [5].

Such arrays are responsible for generation of an excess voltage observed in numerous experiments on mesoscopic CDW samples (see, e. g., Refs. [7–9]) and were studied in a series of phenomenological theoretical models [5,7,10–13] in which the problem of the charge transformations dynamics remained unresolved. To our knowledge, the only paper in which an attempt was made to devise a self-trapping mechanism in a *1D* CDW conductor, was the Ref. 6. It has been shown in [6] that at low temperatures, $T \ll T_c$, the transfer of conduction electrons to the valence band occurs via instantons which split from a conduction band a level occupied by two electrons and push this level towards the valence band. An instanton interpolates between the initial state:

$$|\mathrm{in}\rangle \equiv |\ 2 \text{ conduction electrons}, \varphi = \text{const}, \Delta = \text{const}\,\rangle$$

and the final one:

$$|f\rangle \equiv |\ \text{no conduction electrons}, \delta\varphi_{\mathrm{in}} = 2\pi, \Delta = \text{const}\rangle\,,$$

and describes the self-trapping stage of conversion or the nucleation of a phase-slip-center (PSC). The instanton mechanism is most efficient at a metal–CDW interface [6], because the instanton action exponentially grows with the distance.

The subsequent evolution of the PSC has not been investigated yet, and it is the aim of this paper to put forward the qualitative microscopic theory of transformation of a trapped electron pair into intrinsically nonlinear phase excitations of CDW.

The scenario of charge transformation is as follows: at time $t \sim \omega^{-1}$, a self-trapped pair of electrons creates the initial phase profile $\delta\varphi_{\mathrm{in}} = 2\pi$ ($|f\rangle$-state) localized on a scale of the Peierls coherence length, $l_{\mathrm{trap}} \sim \xi_0 = \hbar v_F/\Delta$, the length ξ_0 being not the intrinsic scale of the phase Hamiltonian [3,4], thus $\delta\varphi_{\mathrm{in}}$ serves as the initial condition to the phase motion equations. To solve the Cauchy problem, we formulate the exactly solvable model of phase dynamics in a cluster of next-to-nearest neighbor chains and apply the inverse scattering transformation (IST) method. It appears that over the time $t_2 \sim \Delta/(\omega T_c)$, the initial condition $\delta\varphi_{\mathrm{in}}$ transforms into a charged 2π-kink with a core of order $\hbar v_F/T_c$ localized in the same chain and surrounded by dipoles in all the other chains.

For definiteness, let us take the zero temperature and study the conversion of two electrons to a cluster of Z nearest CDW chains which are oriented along the most conducting x direction and occupy the semiaxis $x \geq 0$.

The phase Lagrangian takes the form [3,4]

$$L = \frac{1}{\pi\hbar v_F}\times$$

$$\times\left\{\frac{\Delta^2(\partial\varphi_0/\partial t)^2}{\omega^2} + Z\frac{\Delta^2(\partial\varphi/\partial t)^2}{\omega^2} - \frac{\hbar^2 v_F^2(\partial\varphi_0/\partial x)^2}{4} - \right.$$

$$\left. - Z\frac{\hbar^2 v_F^2(\partial\varphi_0/\partial x)^2}{4} + 2ZT_c^2\cos(\varphi_0 - \varphi)\right\}\,, \quad (3)$$

where φ_0 denotes the phase in a central chain, and φ denotes phases in the nearest ones. At $t = 0$ two electrons pass to a central chain: $\varphi_0(x, t = 0) \neq 0$, $\varphi(x, t = 0) = 0$.

The Cauchy problem must be supplemented with boundary conditions at $t = 0$, see Eqs. (5) below. The initial moment $t = 0$ to the Cauchy problem is defined as the one when the phase configuration $\delta\varphi_{\mathrm{in}}$ escapes from under the autolocalization potential barrier with zero velocity [6]:

$$\frac{\partial\varphi}{\partial t}(t = 0) = 0\ . \quad (4a)$$

As the result of the energy conservation in the process of self-trapping we get

$$2\Delta = \int dx\,\frac{\hbar v_F}{\pi}\left(\frac{\partial\varphi_0}{\partial x}\right)^2\,, \quad (4b)$$

and hence $\frac{\partial\varphi_0}{\partial x}(t = 0) \sim \frac{1}{\xi_0}$.

The compatibility of this initial condition to the Lagrangian (3) needs special comment. The Lagrangian (3) is actually valid when phase gradients are small compared to ξ_0^{-1}, when $|\partial\varphi/\partial x| \sim \xi_0^{-1}$, the modulus and phase dynamics cannot be separated. Thus, when introducing the above initial condition to the phase dynamics equations solely, we suppose the existence of an intermediate region which we cannot describe analytically where the product $\xi_0\,|\partial\varphi_0/\partial x|$ is numerically but not parametrically small.

Minding the above said, we present the model complete set of boundary conditions in a physically plausible form:

$$\frac{\partial\varphi_0}{\partial x}(t = 0) \sim \frac{1}{\xi_0}\,, \quad \frac{\partial\varphi}{\partial x}(t = 0) = 0\,, \quad (5a)$$

$$\int_0^\infty dx\,\frac{\partial\varphi_0}{\partial x}(t = 0) = \delta\varphi_{\mathrm{in}} = 2\pi\,, \quad (5b)$$

$$\varphi_0(x = 0, t = 0) = -2\pi\,,\ \varphi_0(x \to \infty, t = 0) = 0\,, \quad (5c)$$

$$\frac{\partial\varphi_0}{\partial t}(t = 0) = \frac{\partial\varphi}{\partial t}(t = 0)\ . \quad (5d)$$

Introduce new variables $\eta = \varphi_0 - \varphi, \chi = \varphi_0 + Z\varphi$. Now the motion equations read:

$$\frac{\partial^2\chi}{\partial\tau^2} - \frac{\partial^2\chi}{\partial y^2} = 0\,, \quad (6a)$$

$$\frac{\partial^2\eta}{\partial\tau^2} - \frac{\partial^2\eta}{\partial y^2} + (Z+1)\sin\eta = 0 \quad , \qquad (6b)$$

where $\tau = 2T_c \frac{\omega}{\Delta} t$, $y = \frac{4T_c}{\hbar v_F} x$.

It is convenient to make the analytical continuation to the whole axis $-\infty < x < \infty$ recalling, when necessary, that the physically significant results should be studied finally on the semiaxis $0 \le x < \infty$, and represent the boundary conditions in a model form:

$$\frac{\partial\chi}{\partial\tau}(\tau = 0) = \frac{\partial\eta}{\partial\tau}(\tau = 0) = 0 \ , \qquad (7a)$$

$$\frac{\partial\chi}{\partial y}(\tau = 0) = \frac{\partial\eta}{\partial y}(\tau = 0) = f(y) \ , \qquad (7b)$$

where

$$f(y) = \begin{cases} 2f_0 = \dfrac{\pi\Delta}{2T_c} \ , & |y| < \dfrac{4T_c}{\Delta} = l_0 \ , \\ 0 \ , & |y| > l_0 \ . \end{cases} \qquad (8)$$

The charge conservation imposes the topological constriction:

$$\int\limits_0^\infty dy \left(\frac{\partial\varphi_0(y,\tau)}{\partial y} + Z\frac{\partial\varphi(y,\tau)}{\partial y}\right) = \int\limits_0^\infty dy \frac{\partial\chi(y,\tau)}{\partial y} = 2\pi \ . \qquad (9)$$

The solution of the linear equation (6a) takes the form

$$\chi(y,\tau) = \frac{1}{2}\left(F(y-\tau) + F(y+\tau)\right) - 2\pi \ , \qquad (10)$$

where

$$F(z) = \begin{cases} 2\pi + \chi(z,0) \ , & z > 0 \ ; \\ -\chi(|z|,0) - 2\pi \ , & z < 0 \ . \end{cases} \qquad (11)$$

To solve the Cauchy problem for the sine-Gordon (SG) equation (6b) we use the IST [14]. Within the IST approach, the SG equation is related to the linear scattering problem:

$$\hat{L}(\eta, \eta_{\bar\tau}; \lambda)\Psi(\xi, \bar\tau; \lambda) = 0 \qquad (12)$$

for the auxiliary spinor Jost function

$$\Psi(\xi, \bar\tau; \lambda) = \begin{pmatrix}\Psi_1 \\ \Psi_2\end{pmatrix} \ ,$$

where λ is the spectral parameter which takes real positive values and $\xi = y/(Z+1)^{1/2}$, $\bar\tau = \tau/(Z+1)^{1/2}$. The operator $\hat{L}$ takes the form

$$\hat{L} = \hat{I}\frac{\partial}{\partial\xi} - $$
$$- \frac{i}{2}\left[\left(\lambda - \frac{1}{4\lambda}\cos\eta\right)\hat\sigma_3 - \frac{\hat\sigma_2}{4\lambda}\sin\eta + \frac{\hat\sigma_1}{2}(\eta_\xi - \eta_{\bar\tau})\right] , \qquad (13)$$

where $\hat\sigma_\alpha$ $(\alpha = 1, 2, 3)$ are the Pauli matrices, and $\hat{I}$ is the unit matrix.

To construct the solution, one has to calculate the Jost coefficients and to find zeros of the reflection coefficient [14]. Consider the eigenfunctions $\Psi(\xi, \lambda)$ with the asymptotes at $\xi \to -\infty$

$$\Psi_- = \begin{pmatrix} 0 \\ e^{-i\Lambda\xi}\end{pmatrix} \ , \qquad (14)$$

where $\Lambda = \lambda - 1/(4\lambda)$ and at $\xi \to \infty$

$$\Psi_+ = \begin{pmatrix} b(\lambda)\, e^{i\Lambda\xi} \\ a(\lambda)\, e^{-i\Lambda\xi}\end{pmatrix} \ . \qquad (15)$$

The functions $b(\lambda)$ and $a(\lambda)$ are the Jost coefficients; zeros of $a(\lambda)$ define the solutions to the SG equation.

To calculate the initial Jost coefficients, we put in (13) $\cos\eta(\xi, 0) = 1$ which is justified by the inequality $T_c \ll \Delta$. We get

$$a(\lambda, 0) = \exp(i\Lambda l_0)\left(\cos kl_0 - i\frac{\Lambda}{k}\sin kl_0\right) \ , \qquad (16)$$

$$b(\lambda, 0) = i\frac{f_0}{k}\sin kl_0 \ , \qquad (17)$$

where $k = (\Lambda^2 + f_0^2)^{1/2}$.

The spectral equations $a(\lambda, 0) = 0$ was analyzed in the Ref. 15 where it has been shown that the condition $l_0 f_0 = \pi$ (see the Eq. (8)) corresponds to pair of kinks moving in opposite directions. The kink on the semiaxis $x \ge 0$ is the only physically relevant for us. Its asymptote at $t \to \infty$ is

$$\eta(x,t) =$$
$$= -4\tan^{-1}\exp\left\{-\frac{x - vt}{d(Z+1)^{1/2}(1 - v^2/C_0^2)^{1/2}}\right\} , \qquad (18)$$

where $d = \hbar v_F/2T_c$, $C_0 = v_F\hbar\omega/\Delta$ and

$$v = C_0 \times$$
$$\times \left\{1 - \frac{8(Z+1)^{1/2}T_c/\pi\Delta}{1 + \left[1 - \left(8(Z+1)^{1/2}T_c/\pi\Delta\right)^2\right]^{1/2}}\right\} . \qquad (19)$$

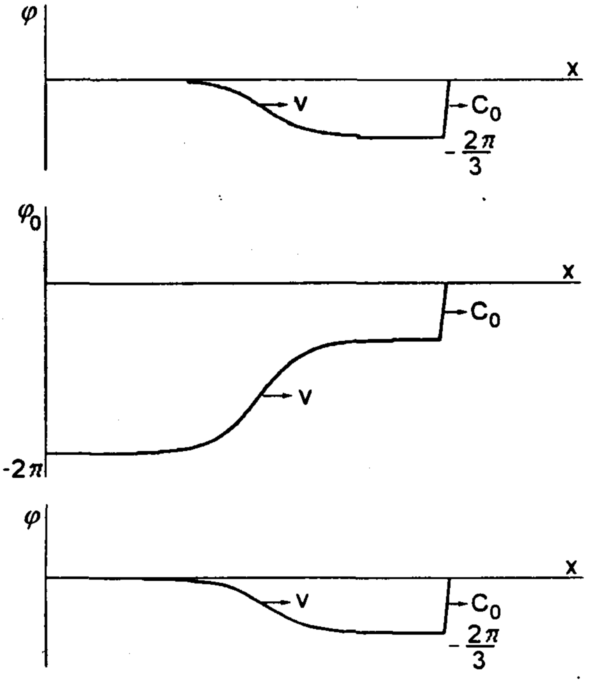

Fig. 1. Phase distribution in a central and neighboring chains, $Z = 2$.

For the parameters of TaS_3 [2], $v \approx 0.98C_0$.

The solution (18) itself satisfies the topological condition

$$\delta\eta = \eta(x \to \infty, t) - \eta(x = 0, t) = 2\pi \ , \qquad (20)$$

which means that the electric charge of self-trapped electrons remains localized in a central chain at arbitrary time. Indeed, combining the Eq. (20) and the Eq. (9) we get

$$\delta\varphi_0 = 2\pi \text{ and } \delta\varphi = 0 \ . \qquad (21)$$

All the other chains contain dipoles with charges

$$q_{\text{dip}} = \pm \frac{2e}{Z+1} \ , \qquad (22)$$

the length of a dipole is proportional to $l_{\text{dip}} \sim \delta v = C_0 \mp v$.

Phase distribution for TaS_3 ($Z = 2$) is shown schematically in Fig. 1.

The above presented solution of the Cauchy problem, though physically transparent, leaves certain feeling of discontent because of two reasons: it is accessible only for a model boundary condition (7b), (8). Besides, the IST method cannot even give an estimate for the time at which the asymptote (18) is reached.

Below we show qualitively that the principal results (21) are, in fact, insensitive to a specific shape (8) of $f(x)$ and only depend on the topological constrictions (5b), (5c). We also show that the time of the steady-kink-velocity formation is of the order ω^{-1} and weakly depends on the shape of initial phase profile. The time of a 2π-kink steady profile formation is of order of $\Delta/(\omega T_c) \gg \omega^{-1}$.

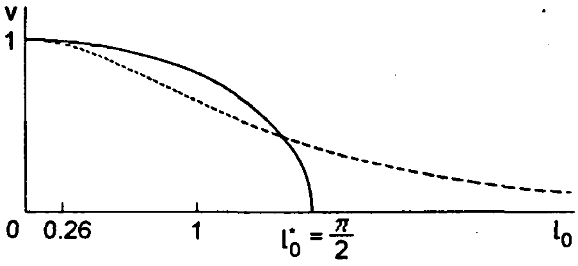

Fig. 2. Dependence of a kink velocity on initial condition. Solid line: result of the IST analysis; dashed line: trial function (23).

Consider the one parameter two-soliton solution to the SG equation [16]:

$$\eta_R(\xi, \tau) = -4 \tan^{-1} \left(\frac{\cosh \left(U\tau/(1-U^2)^{1/2}\right)}{U \sinh \left(\xi/(1-U^2)^{1/2}\right)} \right) \ , \qquad (23)$$

where $U = v/C_0$, which obeys the initial conditions:

$$\begin{aligned} \eta_R(\xi = +0, \tau = 0) &= -2\pi \ , \\ \eta_R(\xi \to +\infty, \tau = 0) &= 0 \ . \end{aligned} \qquad (24)$$

To connect U with the initial space derivative, put $\eta_R(\xi = l_0, \tau = 0) = -\pi$ which gives

$$l_0 = (1 - U^2)^{1/2} \tan^{-1}(1/U) \ . \qquad (25)$$

For TaS_3 parameters, $l_0 \approx 0.26$, we obtain $v \cong 0.96C_0$ in an excellent agreement with the IST results (Fig. 2).

It is convenient to define the time of establishing the asymptotically steady velocity, τ_∞, as the one when the time derivative of a profile at a point ξ equals $U/2$, i.e.

$$\left.\frac{d\xi}{d\tau}\right|_{\tau = \tau_\infty} = \frac{U}{2} = = \frac{\sinh\left(U\tau_\infty/(1-U^2)^{1/2}\right)}{\left[1 + \left(\cosh\left(U\tau_\infty/(1-U^2)^{1/2}\right)U^{-1}\right)^2\right]^{1/2}} \ . \qquad (26)$$

We get from (26)

$$\tau_\infty = \frac{(1-U^2)^{1/2}}{U} \operatorname{arcsinh} \left(\frac{1+U^2}{3} \right)^{1/2} \qquad (27)$$

Combining (27) and (25) we arrive at $\tau_\infty \sim l_0$ ($\tau_\infty \sim 1/\omega$).

Mention should be made, at least qualitatively, how three-dimensional effects modify the results obtained within the framework of the model (3) which, though takes into account the interaction with neighboring chains, is essentially one-dimensional one. As our model (3) mathematically is closely related to the model of a crowdion in $3D$ elastic medium, we can use the results for crowdion [17].

Numerical analysis [17] shows the existence of two scales in the core of a localized charge density ρ, resulting from the nonlocal nature of the model. At large distances $x >> l_c \sim 30d$ ($d = \hbar v_F / 2T_c$), the exponential decrease in the density ρ changes to the power-law relationship $\rho \sim (l_c / x)^3$.

Whereas the density peculiar to a charged chain is of order of $\rho_0 \sim e/d$, the charge densities in neighboring chains are of order of $\rho_* \sim 10^{-2} e/d$ and the scale of a dipole field is of order of $l_d \sim 10d$.

Furthermore, the dynamics of a charge formation in a $3D$ case is more complicated than in a $1D$ model. There are two different characteristic velocities in a $3D$ medium: the longitudinal one C_0, and the transverse one $C_\perp \sim (T_c / \varepsilon_F) C_0 << C_0$. The charge moving with the velocities v in the interval $C_\perp < v < C_0$, produces the Cherenkov radiation with the radiative force [18]

$$F \sim \left(v^2 - C_\perp^2\right) \left(\frac{T_c}{\varepsilon_F}\right)^4 . \qquad (28)$$

It follows from the Eq. (28) that the charge which comes into being with the initial velocity $v \cong C_0$ loses its velocity to the point $C_\perp$ over distance $l_h \sim \xi_0 (\varepsilon_F / T_c)^3$ during the time $t_h \sim (1/\omega)(\varepsilon_F / T_c)^3$. This radiative effect can be speculatively related to the «narrow band noise» problem [1,2].

And finally, note that in a case of a static kink, the dipole field in neighboring chains transforms to a quadrupole one [17].

This work was partially supported by the Joint Grants of the Goverment of Ukraine and the International Science Foundation, ISF U2K200, ISF U2I200, and the grant INTAS-98-1662.

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