Collective excitation of charge-density waves in quasi-one-dimensional structures

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Oscillations of the phase of the order parameter are considered in quasi-one-dimensional systems that undergo a Peierls structural transition. Their spectrum is calculated with allowance for the effects of the Coulomb interaction of the charge-density wave (CDW) on different chains and within a single chain. It is shown that the interaction of the CDW with charged impurities leads to pinning of the wave. Nonlinear excitations of CDW of the soliton type are considered. CDW interaction on neighboring chains leads to a binding of solitons and antisolitons into pairs that play the role of defects in the CDW structure.

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Recent years have seen an increased interest in the study of the properties of quasi-one-dimensional systems, particularly systems that undergo a Peierls structural transition.[1] This interest is stimulated by the experimental observation of a Peierls transition in compounds of the type $K_2Pt(CN)_4Br_{0.3}3H_2O$(KCP) (Refs. 2–4) and TTF−TCNQ (Refs. 5 and 6), and also the possibility of observing anomalous conductivity connected with displacement of the charge-density wave (CDW) that occurs in the transition.[7–9] This latter property of such systems turns out to be closely connected with collective excitations of CDW (Refs. 9 and 10) which are being actively studied experimentally.[11–12]

The present paper is devoted to a consideration of the spectrum of the collective excitations of CDW in the low-temperature region, on the basis of a generalized semiphenomenological model proposed in Refs. 13 and 14. The model is generalized from the pure one-dimensional case to include the quasi-one-dimensional case, and the influence of the impurities and of commensurability effects is investigated. The possible existence of new modes of the collective-excitation spectrum of the soliton type in a purely one-dimensional model is considered, with a qualitative allowance for three-dimensional and Coulomb effects.

The model is quite general, and the main results may be applicable to CDW that are not of the Peierls type.

1. FORMULATION OF THE MODEL AND EXCITATION SPECTRUM IN THE LINEAR APPROXIMATION

We consider a quasi-one-dimensional system at temperatures much lower than the Peierls-transition point [$T_p \sim 120$°K for KCP (Ref. 4), $T_p = 54$°K for TTF–TCNQ (Ref. 6)]. In each chain there exists a nonzero order parameter of the CDW,

$$\operatorname{Re}\Psi(x) = \operatorname{Re}\{\Delta \exp[iQx + \Phi]\}, \tag{1}$$

where Δ is the amplitude of the order parameter and is connected with the gap in the spectrum of the single-electron excitations of the Peierls phase[1]; Φ is the phase shift of the order parameter and determines the position of the CDW relative to the immobile coordinate system[9]; $Q = 2p_F$, where p_F is the Fermi momentum of the electrons and is connected with their linear density by the relation $p_F = (\pi/2)n$.

The collective excitations of the CDW correspond to the fact that in (1) the amplitude and phase $\Delta(xt)$ and $\Phi(xt)$ become coordinate and time functions that are different from the equilibrium values Δ and Φ. We consider henceforth only excitations of the phase shift of the order parameter,[14] which can be regarded in first-order approximation independently of the amplitude oscillations,[9] at least at sufficiently low temperatures $T \ll T_p$. This question was considered in greater detail by Brazovskii and Dayaloshinskii.[10] It will be assumed that $\Phi(xt)$ is a sufficiently smooth function of the coordinate and of the time.

From the form of (1) it is easily seen[8,14] that the dependence of the CDW phase on the time means displacement of the wave along the chain with velocity

$$v_1 = -\frac{1}{Q}\frac{\partial\Phi}{\partial t}. \tag{2}$$

Analogously, the presence of a spatial gradient of the phase means local variation of the Fermi momentum of the electrons

$$\delta p_F = \frac{1}{2}\frac{\partial\Phi}{\partial x}; \tag{3}$$

and then the excitation of $\Phi(xt)$ corresponds to a linear energy density

$$E = \frac{n_s}{2m}(\delta p_F)^2 + \frac{1}{2}m^* n_s v_s^2 = \frac{n_s m^*}{Q^2}\left\{\frac{1}{2}\left(\frac{\partial\Phi}{\partial t}\right)^2 + \frac{s^2}{2}\left(\frac{\partial\Phi}{\partial x}\right)^2\right\}, \tag{4}$$

where n_s is the linear density of the electrons that move together with the CDW; m* is the effective mass connected with the motion of the CDW (Refs. 13 and 14); m is the effective mass of the electron in the chain

$$s^2 = \frac{p_F^2}{mm^*}. \tag{5}$$

The phenomenological parameters n_s and m* can be determined from the microscopic theory and depend on the concrete model whereby the CDW is produced. In the simplest theory of Peierls transitions at $T \ll T_p$ we have[9,13,14]

$$\left.\begin{aligned} n_s &\approx n, \\ \frac{m^*}{m} &= 1 + \frac{4\Delta^2}{\lambda\omega_Q^2} \simeq \frac{4\Delta^2}{\lambda\omega_Q^2}, \end{aligned}\right\} \tag{6}$$

where n is the total linear density of the electrons in the chain, Δ is the gap in the electron spectrum at T = 0, ω_Q^2 is the characteristic frequency of the "bare" phonon ($\omega_Q \sim \theta_D$ is the Debye temperature), and λ is the dimensionless constant of the electron–phonon interaction. Usually $m^* \gg m$, for example $m^* \approx 10^3 m$ for KCP (Refs. 11 and 13).

It follows from Refs. 1 and 4 that the effective Lagrangian of a CDW on an isolated chain is

$$\mathcal{L}_0 = nm^*\frac{1}{Q^2}\left\{\frac{1}{2}\left(\frac{\partial\Phi}{\partial t}\right)^2 - \frac{1}{2}s^2\left(\frac{\partial\Phi}{\partial x}\right)^2\right\}. \tag{7}$$

The derivation of such a Lagrangian from the microscopic theory is given in Ref. 10. This leads to the standard wave equation

$$\frac{\partial^2\Phi}{\partial t^2} - s^2\frac{\partial^2\Phi}{\partial x^2} = 0, \tag{8}$$

which coincides, when account is taken of (2) and (3), with the hydrodynamic equation of motion[14]

$$nm\frac{\partial v_s}{\partial t} = -n\frac{m}{m^*}\nabla\mu, \tag{9}$$

where μ is the chemical potential (Fermi energy) of the electrons, and the factor m/m* determines the fraction of the CDW mass carried by the electrons. The spectrum of the CDW phase oscillations under the foregoing assumptions takes the form

$$\omega^2 = s^2q^2. \tag{10}$$

which corresponds to the Goldstone mode of Lee, Rice, and Anderson, corresponding to the Frohlich "superconductivity" in the considered model.[9]

Our purpose is to consider the role of various interactions that are not taken into account by the zero-order Lagrangian (7). These include primarily the interaction of the CDW on various chains in a quasi-one-dimensional systems, the role of Coulomb effects in one chain, and interactions with charged impurities.

The Peierls CDW corresponds to modulation of the density of an electron charge along the chain, in the form[9]

$$\rho(x) = ne\frac{\Delta}{\lambda E_F}\cos(Qx + \Phi), \tag{11}$$

so that this chain produces around itself an electrostatic field with a potential

$$\varphi(r_\perp x) = 2ne\frac{\Delta}{\lambda E_F}\cos(Qx + \Phi)\,K_0(Qr_\perp), \tag{12}$$

where e is the electron charge, E_F is the Fermi energy of the chain, $r_\perp$ is the radial distance from the chain, and $K_0(x)$ is a modified Bessel function. Accordingly, in a system of chains forming a regular lattice in a plane orthogonal to the chains, with a lattice constant $r_\perp = b$, an elec-

trostatic interaction energy is produced (per unit length of the system)

$$U = nm^* \frac{1}{Q^2} \sum_{\mathbf{n}} \sum_{\langle \mathbf{m} \rangle} \omega_c^2 \cos(\Phi_{\mathbf{n}} - \Phi_{\mathbf{m}}), \tag{13}$$

$$\omega_c^2 = \omega_Q^2 \left(\frac{\omega_p}{4E_F}\right)^2 \frac{(Qr_\perp)^2}{2\pi\lambda\varepsilon_\perp} K_0(Qr_\perp)|_{r_\perp = b}, \tag{14}$$

where $\mathbf{n}$ and $\mathbf{m}$ determine the positions of the chains in the plane lattice, ω_p is the plasma frequency of the electrons, and $\varepsilon_\perp$ is the dielectric constant of the system in a direction transverse to the chains. It suffices to take into account in (13) the nearest-neighbor interaction, since $K_0(Qr_\perp)$ is exponentially small when $Qr_\perp \gg 1$. The interaction (13), in particular, causes the CDW on the neighboring chains to be conveniently aligned in such a way that their phases differ by π, as is indeed observed experimentally in KCP (Ref. 4).

The Lagrangian of the system now takes the form[1)]

$$\mathcal{L} = nm^* \frac{1}{Q^2} \sum_{\mathbf{n}} \frac{1}{2} \left\{ \left(\frac{\partial \Phi_{\mathbf{n}}}{\partial t}\right)^2 - s^2 \left(\frac{\partial \Phi_{\mathbf{n}}}{\partial x}\right)^2 \right\} - \sum_{\mathbf{n}} \sum_{\langle \mathbf{m} \rangle} \omega_c^2 \{1 + \cos(\Phi_{\mathbf{n}} - \Phi_{\mathbf{m}})\}. \tag{15}$$

We consider a linearized variant of the theory, corresponding to $\Phi_{\mathbf{n}} \ll 1$, $\Phi_{\mathbf{m}} \approx \pi$, so that (15) goes over into

$$\mathcal{L} \approx nm^* \frac{1}{Q^2} \left\{ \sum_{\mathbf{n}} \frac{1}{2} \left[\left(\frac{\partial \Phi_{\mathbf{n}}}{\partial t}\right)^2 - s^2 \left(\frac{\partial \Phi_{\mathbf{n}}}{\partial x}\right)^2 - 2\omega_c^2 \Phi_{\mathbf{n}}^2 \right] + \omega_c^2 \sum_{\mathbf{n}} \sum_{\langle \mathbf{m} \rangle} \Phi_{\mathbf{n}} \Phi_{\mathbf{m}} \right\}, \tag{16}$$

where all the $\Phi_{\mathbf{n}}$, $\Phi_{\mathbf{m}}$ now denote small deviations from the equilibrium values. The corresponding equations of motion take the form

$$\frac{\partial^2 \Phi_{\mathbf{n}}}{\partial t^2} - s^2 \frac{\partial^2 \Phi_{\mathbf{n}}}{\partial x^2} - 4\omega_c^2 \Phi_{\mathbf{n}} = \omega_c^2 \sum_{\langle \mathbf{m} \rangle} \Phi_{\mathbf{m}}. \tag{17}$$

We seek the solution in the form

$$\Phi_{\mathbf{n}}(xt) = \sum_{q\mathbf{q}_\perp} \Phi_{q\mathbf{q}_\perp \omega} e^{i(qx + \mathbf{q}_\perp \mathbf{n} - \omega t)} \tag{18}$$

and obtain the spectrum

$$\omega^2 = s^2 q^2 + 2\omega_c^2 \{2 - \cos q_\perp^x b - \cos q_\perp^y b\}, \tag{19}$$

where the lattice of chain is assumed for simplicity to be quadratic (b is the lattice constant). For $q_\perp = 0$ we have again the acoustic spectrum (10). Thus, the interaction of the chains does not lead to pinning of the CDW.

We now take into account the Coulomb effect in an individual chain. The phase gradient, according to (3) and according to the connection between the Fermi momentum and the electron density, signifies local variation of the charge density

$$\delta\rho = \frac{e}{\pi} \frac{\partial \Phi}{\partial x}, \tag{20}$$

which produces a corresponding electric field in the chain. To take this circumstance into account it is necessary to solve in place of (17) a coupled system of equations of motion

$$\frac{\partial^2 \Phi_{\mathbf{n}}}{\partial t^2} - s^2 \frac{\partial^2 \Phi_{\mathbf{n}}}{\partial x^2} + 4\omega_c^2 \Phi_{\mathbf{n}} = \omega_c^2 \sum_{\langle \mathbf{m} \rangle} \Phi_{\mathbf{m}} + \frac{\pi n e}{m^* \varepsilon_b} \frac{\partial \varphi_{\mathbf{n}}}{\partial x}, \tag{21}$$

which take into account the action of the electric field with potential $\varphi_{\mathbf{n}}$, defined by a differential-difference Poisson equation

$$-\frac{\partial^2 \varphi_{\mathbf{n}}}{\partial x^2} - \frac{1}{b^2} \sum_{i = y, z} [\varphi_{\mathbf{n}+b_i} - 2\varphi_{\mathbf{n}} + \varphi_{\mathbf{n}-b_i}] = 4e \frac{\partial \Phi_{\mathbf{n}}}{\partial x} \sum_{\varkappa_\perp} e^{i\varkappa_\perp \mathbf{n}}. \tag{22}$$

The last term in (21) corresponds to replacement of the chemical potential in (9) by the electrochemical potential. Here ε_l is the dielectric constant due to electron transitions through the Peierls gap

$$\varepsilon_b = 1 + \frac{\omega_p^2}{6\Delta^2}. \tag{23}$$

In (22), $\varkappa_\perp$ are the reciprocal-lattice vectors of the chains. We seek the solution for $\Phi_{\mathbf{n}}(xt)\Phi_{\mathbf{n}}(xt)$ in the form (18) and in analogous form for $\varphi_{\mathbf{n}}(xt)$. Solving the corresponding secular equation, we obtain the spectrum of the excitations

$$\omega^2 = s^2 q^2 + \frac{\omega_p^{*2}}{\varepsilon_b} \frac{q^2}{q^2 + \frac{2}{b^2}[2 - \cos q_\perp^x b - \cos q_\perp^y b]} + 2\omega_c^2 [2 - \cos q_\perp^x b - \cos q_\perp^y b], \tag{24}$$

where $\omega_p^{*2} = 4\pi ne^2/m^*$. The Coulomb effects lead to a finite frequency $\omega_p^{*2}/\varepsilon_b \simeq (3/2)\lambda\omega_Q^2$ of the phase oscillations at $q_\perp = 0$; at $q_\perp b \ll 1$ we have

$$\omega^2 = \frac{\omega_p^{*2}}{|\varepsilon_b|} \cos^2\theta + s^2 q^2 + \omega_c^2 b^2 q^2, \tag{25}$$

where $\operatorname{tg}\theta = q_\perp/q$. For $\mathbf{q}_\perp = (\pi/b, \pi/b)$ we have

$$\omega^2 = 8\omega_c^2 + \left\{ s^2 + \frac{1}{8} b^2 \frac{\omega_p^{*2}}{\varepsilon_b} \right\} q^2. \tag{26}$$

The spectrum (24) constitutes a natural generalization of the results of Refs. 9 and 14 to the case of quasi-one-dimensional systems. The displacement of the atoms in the n-th chain following excitation of small oscillations of the order-parameter phase shift is proportional to

$$u_{\mathbf{n}} \sim \exp\left\{ iQx + i\frac{\pi}{b}\mathbf{n} + i\Phi_{q\mathbf{q}_\perp \omega} e^{iqx + i\mathbf{q}_\perp \mathbf{n} - i\omega t} \right\} \approx e^{iQx + i\frac{\pi}{b}\mathbf{n}} + i\Phi_{q\mathbf{q}_\perp \omega} e^{i(Q+q)x + i\left(\frac{\pi}{b} + \mathbf{q}_\perp\right)\mathbf{n} - i\omega t}. \tag{27}$$

Thus, the phase oscillations with wave vector $\mathbf{q} = (q, q_\perp)$ correspond to excitation of phonons with wave vector $(Q + q, \pi/b + q_\perp^y, \pi/b + q_\perp^z)$, so that the study of the phonon spectrum at the point $(Q, \pi/b, \pi/b)$ corresponds to a study of phase oscillations with $\mathbf{q} = (0, 0, 0)$. As seen

from (27), these oscillations correspond to antiparallel displacements of the atoms in the neighboring chains.[15] Analogously, the phonon spectrum at the point (Q, 0, 0) is connected with the phase oscillations with q = (0, π/b, π/b) corresponding to parallel displacements in the neighboring chains.

Low-frequency optical phonons were observed in Ref. 12 in KCP at the points (Q, π/b, π/b) and (Q, 0, 0), which can tentatively be interpreted as connected with oscillations of the order-parameter phase shift. The weak dispersion of these phonons is explained by the gap-like character of their spectrum (an unjustified comparison with the acoustic spectrum (10) was made in Ref. 12). At the same time, the equality of the phonon frequencies observed at the points (Q, π/b, π/b) and (Q, 0, 0) remains unexplained. We emphasize that the absence of total three-dimensional ordering in KCP (Ref. 4), which is apparently due to disorder effects, can lead to a discernible change of the results obtained above, which are valid, strictly speaking, only for a system consisting of one-dimensional chains of the same type, without the internal disorder inherent in systems of the KCP type.

2. EFFECT OF IMPURITIES ON THE CDW EXCITATION SPECTRUM

Lee, Rice, and Anderson[9] have advanced arguments favoring the assumption that the interaction of CDW with charged impurities converts the acoustic-type phase-oscillation spectrum (10) into a spectrum with a gap, meaning a pinning of the CDW on the impurities and elimination of the Frohlich "superconductivity." At the same time, it was stated in Ref. 16 that the interaction of CDW with random impurities does not lead to pinning. There is as yet no calculation of the spectrum of the phase oscillations of the CDW with allowance for the interaction with the impurities in any concrete model. We present below such a calculation in the considered semiphenomenological theory.

We consider a system of charges disposed in random fashion along a chain with CDW, at a distance $r_\perp$ from the chain. Such a situation is apparently realized in KCP, where the acceptor atoms (of the Br type) are randomly arranged in the system along Pt chains.[1] The impurity charge density

$$\rho(x)=\sum_j e\delta(x-x_j), \tag{28}$$

where x_j are the impurity coordinates, interacts with the CDW potential (12), so that the interaction energy per unit length of the system is

$$U_{\text{imp}}=nm^*\frac{1}{Q^2}\omega_{\text{imp}}^2\frac{1}{N}\sum_j\{\cos(Qx_j+\Phi)\}, \tag{29}$$

where

$$\omega_{\text{imp}}^2=\frac{\omega_p^{*2}}{4\pi\lambda\nu\varepsilon_\perp}\left(\frac{\Delta}{E_F}\right)(Qr_\perp)^2K_0(Qr_\perp), \tag{30}$$

N is the number of atoms in the chain and ν is the number of conduction electrons per atom.

We consider again the linearized theory ($\Phi \ll 1$). The Lagrangian of the system takes the form

$$\mathcal{L}=nm^*\frac{1}{Q^2}\left\{\frac{1}{2}\left(\frac{\partial\Phi}{\partial t}\right)^2-\frac{s^2}{2}\left(\frac{\partial\Phi}{\partial x}\right)^2+\omega_{\text{imp}}^2\frac{1}{N}\sum_j\sin Qx_j\Phi+\omega_{\text{imp}}^2\frac{1}{N}\sum_j\cos Qx_j\Phi^2\right\}. \tag{31}$$

The equations of motion are given by

$$\frac{\partial^2\Phi}{\partial t^2}-s^2\frac{\partial^2\Phi}{\partial x^2}=\omega_{\text{imp}}^2\frac{1}{N}\sum_j\sin Qx_j+\omega_{\text{imp}}^2\frac{1}{N}\sum_j\cos Qx_j\Phi. \tag{32}$$

In a system with impurities

$$\Phi=\Phi(xt;\ \{x_j\}) \tag{33}$$

is the functional of the impurity positions. On the other hand, the phase shift, as a component of the order parameter, is a thermodynamic quantity and must be averaged over the ensemble of random impurity configurations. Averaging (32), we obtain

$$\left(\frac{\partial^2}{\partial t^2}-s^2\frac{\partial^2}{\partial x^2}\right)\langle\Phi\rangle=\omega_{\text{imp}}^2\left\langle\frac{1}{N}\sum_j\cos Qx_j\Phi\right\rangle. \tag{34}$$

This gives rise in natural fashion to a chain of equations expressed in terms of the Fourier components in the form

$$(-\omega^2+s^2q^2)\langle\Phi_{q\omega}\rangle=\omega_{\text{imp}}^2\left\langle\frac{1}{N}\sum_j\cos Qx_j\Phi\right\rangle_{q\omega}, \tag{35}$$

$$\left(-\omega^2+s^2q^2\right)\left\langle\frac{1}{N}\sum_j\cos Qx_j\Phi\right\rangle_{q\omega}$$
$$=\omega_{\text{imp}}^2\left\langle\frac{1}{N^2}\sum_j\sin Qx_j\sum_i\cos Qx_i\right\rangle\delta(\omega)\delta(q)$$
$$+\omega_{\text{imp}}^2\left\langle\frac{1}{N^2}\sum_j\cos Qx_j\sum_i\cos Qx_i\Phi\right\rangle_{q\omega}. \tag{36}$$

Carrying out in (36) a very simple decoupling in the impurity correlators, we obtain (at $\omega \neq 0$, $q \neq 0$)

$$\left\{-\omega^2+s^2q^2+\frac{\omega_{\text{imp}}^4}{\omega^2-s^2q^2}\frac{1}{2}S(Q)\right\}\langle\Phi_{q\omega}\rangle=0, \tag{37}$$

where

$$S(Q)=\frac{1}{N^2}\left\langle\sum_{ij}e^{iQ(x_i-x_j)}\right\rangle \tag{38}$$

is the structure factor of the impurity positions. From (37) follows the phase-oscillation spectrum

$$\omega^2=\left\{\frac{1}{2}S(Q)\right\}^{1/2}\omega_{\text{imp}}^2+s^2q^2. \tag{39}$$

For random impurities S(Q) is equal to the impurity

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concentration c_{imp}. Thus, the impurities lead to pinning of the CDW, the gap in the spectrum being

$$\omega_T^2 = \left\{\frac{1}{2} c_{imp}\right\}^{1/2} \omega_{imp}^2. \tag{40}$$

The foregoing analysis is valid for sufficiently low impurity concentrations, which do not influence substantially the Peierls transition itself[17] and which allow the decoupling carried out above. The allowance for the quasi-one-dimensionality and for the Coulomb effects is in the same manner as above; leaving out the calculations, we indicate that as the result the gap ω_T^2 is simply added to the right-hand side of expression (19) or (25). The gap in the spectrum is different from zero at arbitrary q and $q_\perp$.[2)] It is possible that the equality of the phonon frequencies at the points (Q, π/b, π/b) and (Q, 0, 0), which was observed in Ref. 12, is due to the dominant role of the impurities in the formation of the gap.

3. EFFECTS OF COMMENSURABILITY AND NONLINEAR EXCITATIONS

The existence of a Goldstone mode with a spectrum (10) is directly connected with degeneracy of the CDW with respect to the phase Φ. This degeneracy of the CDW having a period that is commensurate with the period of the original chain. In the commensurate case $Q = 2\pi m \cdot (Ma)^{-1}$, where a is the period of the initial chain, and $m < M$ are integers. The CDW energy then acquires a comensurability term[18,14,9]

$$U_{comm} \sim \Delta^M \cos M\Phi. \tag{41}$$

The proper Lagrangian of one chain takes the form

$$\mathcal{L} = \mathcal{L}_0 + nm^* \frac{1}{Q^2} \frac{\omega_T^2}{M^2} (\cos M\Phi - 1), \tag{42}$$

where[9,14]

$$\omega_T^2 \sim \lambda M^2 \omega_Q^2 \left(\frac{\Delta}{E_F}\right)^{M-2}. \tag{43}$$

In the linear approximation we can confine ourselves to expansion of cos MΦ up to quadratic terms, and obtain the spectrum of the phase oscillations in the form[9]

$$\omega^2 = \omega_T^2 + s^2 q^2. \tag{44}$$

Thus, the commensurability effects lead to a pinning of the CDW.

The nonlinear Lagrangian (42) leads to an equation of motion of the sine-Gordon type

$$\frac{\partial^2 \Phi}{\partial t^2} - s^2 \frac{\partial^2 \Phi}{\partial x^2} = -\frac{\omega_T^2}{M^2} \sin M\Phi, \tag{45}$$

for which an extensive spectrum of classical and quantum solutions has been obtained.[19] In addition to the branch corresponding to the linear oscillations of Φ near zero (44), it is possible to excite in the system an arbitrary number of soliton–antisoliton pairs moving with velocity $v < s$

$$\Phi_{sol}(xt) = \frac{4}{M} \operatorname{arc\,tg} \left\{\exp\left(\frac{\omega_T}{s} \frac{x - v/st}{\left(1 - \frac{v^2}{s^2}\right)^{1/2}}\right)\right\}, \tag{46}$$

$$\Phi_{antisol}(xt) = -\Phi_{sol}(xt). \tag{47}$$

The energy of the soliton is expressed by the standard "relativistic" formula

$$E_{sol} = \frac{M_{sol} s^2}{\left(1 - \frac{v^2}{s^2}\right)^{1/2}} = \sqrt{\Delta_{sol}^2 + s^2 p^2}, \tag{48}$$

where the mass M_{sol} ($\Delta_{sol} = M_{sol} s^2$, p is the soliton moment), in the quasiclassical (WKB) approximation (Refs. 18 and 19)[3)], using the parameters of our model, is equal to

$$M_{sol} = nm^* \frac{1}{Q^2} \frac{8\omega_T}{\gamma s} = \frac{4}{\pi} \frac{\omega_T}{s p_F} m^* \frac{1}{\gamma}, \tag{49}$$

where γ is the renormalized coupling constant, equal in the present model to

$$\gamma = \frac{M^2}{1 - \frac{M^2}{8\pi}}. \tag{50}$$

In classical soliton theory we have $\gamma = M^2$. The possible existence of soliton excitations in CDW of the Peierls type was considered in the classical approximation in a recent paper.[28] The form of the soliton solution as a function of x (at v = 0) is shown in Fig. 1. In a region having linear dimensions of the order of

$$\xi_{sol} \approx \frac{s}{\omega_T} \tag{51}$$

(the soliton dimensions) the gradient of the phase differs effectively from zero, i.e., in accordance with (20), there is an excess charge density

$$\delta\rho_{sol} = \frac{2}{M} \frac{e}{\pi} \frac{\omega_T}{s} \operatorname{ch}^{-1} \frac{\omega_T}{s} x; \tag{52}$$

from which it is clear that the soliton carries an electric charge

$$Q_{sol} = \frac{4}{M} e. \tag{53}$$

Antisoliton carry a charge of opposite sign. The motion of the solitons produces a current density [see (3)]

$$j_{sol}(xt) = -\frac{ne}{Q} \Phi_{sol}(xt) = \delta\rho_{sol}(x)\, v. \tag{54}$$

Solitons and antisolitons can be produced only in pairs and are subject to Fermi statistics.[21]

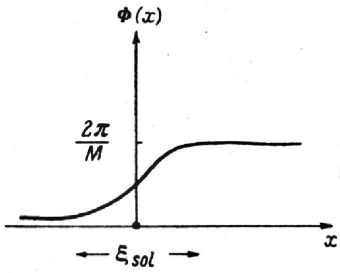

FIG. 1. Change of phase in the region of the soliton solution.

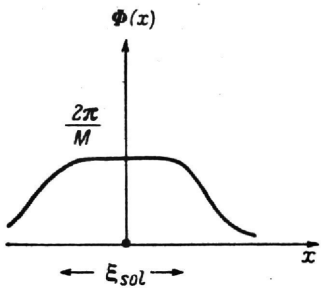

FIG. 2. Change of phase in the region of the bound soliton–antisoliton state.

It is easily seen that the considered model is equivalent to a simple generalization of a one-dimensional dislocation after Frenkel' and Kontorova[22,23], dealing with the motion of a chain of "atoms" and mass m* in a periodic field of a "substrate" produced by the commensurability effects. In this sense, solitons constitute "dislocations" in the CDW lattice.

In addition to solitons, the model under consideration admits of spectrum branches corresponding to bound soliton–antisoliton states, which have not been considered in Ref. 20. Such a "doublet" solution of (45) in the rest system (v = 0) takes the form[18,19]

$$\Phi_d(xt) = \frac{4}{M}\operatorname{arc\,tg}\left\{\varepsilon\frac{\sin\left(\frac{2\pi}{\tau}t\right)}{\operatorname{ch}\left(\varepsilon\frac{2\pi}{\tau}\frac{x}{s}\right)}\right\}, \tag{55}$$

where

$$\varepsilon = \left[\left(\frac{\tau\omega_T}{2\pi}\right)^2 - 1\right]^{1/2}, \quad \tau = \frac{2\pi}{\omega_T\cos\frac{N\gamma}{16}}. \tag{56}$$

Here N = 1, 2, ..., < $8\pi/\gamma$ (Ref. 19) number the stable (in quantum theory) branches of the doublet spectrum. Their masses (gaps in the spectrum) are given in the WKB approximation by[19]

$$M_N = nm^*\frac{1}{Q^2}\frac{16\omega_T}{\gamma s}\sin\left(\frac{N\gamma}{16}\right) = \frac{8}{\pi}\frac{\omega_T}{sp_F}m^*\frac{1}{\gamma}\sin\left(\frac{N\gamma}{16}\right). \tag{57}$$

Taking into account the form of γ(52) and the fact that only M ≥ 3 is meaningful in the considered model (Ref. 9),[4)] we verify that N = 1 for M = 3, and for M > 3 the doublet solutions are unstable.

The doublet solution is shown graphically in Fig. 2. It is obvious that the total charge carried by the doublet is equal to zero, i.e., their motion does not contribute to the constant current. However, a doublet has a dipole moment that oscillates with frequency $2\pi/\tau$, and this could manifest itself in principle in the dielectric constant.

We note that in Ref. 24 an attempt was made to construct doublet-like solutions of an equation of the type (45). However, the approximate formations obtained there have nothing in common with the exact solutions (55) and are apparently unstable. In addition, it is erroneously stated in Ref. 24 that such solutions contribute to the dc conductivity.[5)]

We consider now the degree to which the obtained purely one-dimensional solutions are preserved when account is taken of the Coulomb effects in a single chain, as well as of chain-interaction effects.

The formation of a soliton is not profitable from the point of view of Coulomb effects, since it involves an energy loss $Q^2_{sol}/\xi_{sol}\varepsilon_b$. This energy shortage is immaterial if it is smaller than $M_{sol}s^2$, which leads to the condition $e^2m/\hbar p_F \ll (1/16)\varepsilon_b$, which can be readily satisfied. To take into account the interaction of CDW of neighboring chains it is necessary to consider systems of coupled nonlinear equations.

We present a simple qualitative analysis. The production of a soliton–antisoliton pair on one of the chains leads to a loss of chain-interaction energy [see (13)]

$$U_\perp \sim nm^*\frac{\omega_c^2}{Q^2}\xi\left\{\cos\pi\left(1-\frac{2}{M}\right)+1\right\}, \tag{58}$$

where ξ is the soliton–antisoliton distance. The influence of this loss on the soliton mass is immaterial if $2M_{sol}s^2 \gg U_\perp$, leading to the requirement

$$\xi \ll \frac{16}{M^2}\left(\frac{\omega_T}{\omega_c}\right)^2\xi_{sol}, \tag{59}$$

i.e., the soliton and the antisoliton must be close enough. At the same time it is necessary to have $\xi \gg \xi_{sol}$, for only then can be speak of "individual" solitons. In view of the smallness of ω_T(43) relative to the parameter $(\Delta/E_F)^{M-2} \ll 1$, this condition is difficult to satisfy for the known systems of the type KCP or TTF–TCNQ. At the same time, ω_c decreases exponentially with the increasing distance between the chains (14) in such a way that the situation becomes more favorable in a system of sufficiently separated chains. Owing to (58), the solitons and antisolitons are attracted with a force $\sim nm(\omega_c^2/Q^2)$, and, strictly speaking, are always bound. Let us estimate the minimum dimension of a bound soliton–antisoliton state in the potential well (58)

$$\frac{1}{M_{sol}\xi_b^2} \sim nm^*\frac{\omega_c^2}{Q^2}\xi_b,$$

i.e.,

$$\frac{\xi_b}{\xi_{sol}} \sim M^{2/3}\left(\frac{\omega_T}{\omega_c}\right)^{2/3}\left(\frac{m}{m^*}\right)^{1/3}. \tag{60}$$

Here, too, it is necessary to stipulate $\xi_b > \xi_{sol}$, which

can be readily satisfied. Thus, solutions of the soliton type are not profitable from the point of view of interaction between the chains and can hardly be realized in known systems.[6)] In addition, even under conditions when one can speak of the existence of solitons in individual chains, they are bound into soliton–antisoliton pairs and make no contribution to the conductivity in weak fields,[7)] in contradiction to the statements made in Ref. 21.

We note in conclusion that the loss of energy of the type (58) disappears in a situation corresponding to formation of solitons on all chains in a sample cross section perpendicular to the chains. It can be proved rigorously, however, that such soliton "planes" are not profitable from the point of view of Coulomb effects. For lack of space, this question is not considered here.

In conclusion, the author is grateful to L. N. Bulaevskiĭ for numerous discussions and critical remarks.

[1)]A constant has been added here to make the ground state correspond to $\mathcal{L}=0$, thereby fixing the energy origin.

[2)]Since the phase oscillations are in fact three-dimensional, questions concerning the specific character of the action of impurities in a strictly one-dimensional system are not raised.

[3)]It appears that the WKB mass values used here are exact.[19]

[4)]At M = 2, the phase oscillations of CDW coincide with the amplitude oscillations, which are not considered here.

[5)]In Ref. 24, and in fact also in Ref. 20, they considered an interaction Lagrangian of the type (42) with M = 1. We do not know of any physical mechanisms that lead to such an interaction. It appears that a nonlinear interaction between the chains does not lead to formation of soliton solutions, since it does not ensure pinning of the CDW.

[6)]We note, however, that the binding energies of soliton–antisoliton pairs decrease exponentially with increasing distance between chains.

[7)]A sufficiently strong field $E \sim 2\ 3(M/\pi)(e/r_\perp^2)\omega_c^2/\lambda\omega_Q^2$ will break the soliton–antisoliton pair and their contribution to the conductivity becomes in principle possible. The magnitude of this field also decreases exponentially with increasing distance between chains.

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Erratum: Collective excitation of charge-density waves in quasi-one-dimensional structures [Sov. Phys. Solid State 19, 607–613 (April 1977)]

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The author has made an error in Eqs. (21) and (22) in this article. The correct forms of these equations are

$$\frac{\partial^2\Phi_{\mathbf{n}}}{\partial t^2}-s^2\frac{\partial^2\Phi_{\mathbf{n}}}{\partial x^2}+4\omega_c^2\Phi_{\mathbf{n}}=\omega_c^2\sum_{\langle\mathbf{m}\rangle}\Phi_{\mathbf{m}}+\frac{\pi ne}{m^*}\frac{\partial\varphi_{\mathbf{n}}}{\partial x}, \tag{21}$$

$$-\varepsilon_b\frac{\partial^2\varphi_{\mathbf{n}}}{\partial x^2}-\frac{1}{b^2}\varepsilon_\perp\sum_{i=y,z}[\varphi_{\mathbf{n}+b_i}-2\varphi_{\mathbf{n}}+\varphi_{\mathbf{n}-b_i}]=4e\frac{\partial\Phi_{\mathbf{n}}}{\partial x}\sum_{\mathbf{x}_\perp}e^{i\mathbf{x}_\perp\mathbf{n}}. \tag{22}$$

Equation (24) then becomes

$$\omega^2=s^2q^2+\frac{\omega_p^{*2}}{\varepsilon_b}\frac{q^2}{q^2+\frac{2\varepsilon_\perp}{b^2\varepsilon_b}[2-\cos q_\perp^z b-\cos q_\perp^y b]}+2\omega_c^2[2-\cos q_\perp^z b-\cos q_\perp^y b]. \tag{24}$$

Equation (25) is then valid only for $\varepsilon_\perp=\varepsilon_b$.

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