Domain structure in an electric field in commensurate quasi-one-dimensional conductors

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The jump of the conductivity anisotropy in a transition from a Peierls dielectric into a domain phase is investigated. It is shown that in the domain phase the conductivity-anisotropy parameter can reach anomalously large values $\alpha = \sigma_\perp/\sigma_\parallel \gg 1$. The collective contribution made to the conductivity by the domain superstructure is considered. It turns out that the electrons participating in the collective conductivity constitute a fraction Δ_0/E_F of the total.

INTRODUCTION

The possible existence of solitons, unique quasiparticles with charge 0, $\pm e$ and spin $\pm 1/2$, 0 in quasi-one-dimensional organic conductors has recently attracted much interest and study.[1–3] This problem was investigated in most theoretical papers in a purely one-dimensional formulation (an isolated conducting chain). The mathematical formalism developed within the framework of the one-dimensional approach[3] has made possible the solution of essentially nonlinear problems.

This mathematical formalism was generalized in a natural manner in Ref. 4 to include the more realistic case of quasi-one-dimensional conductors in which, on the one hand, an incommensurate superstructure is made possible by the incomplete superposition of the curved Fermi surfaces (tunnel overlap),[5] and on the other hand, as shown in Ref. 4, this structure can take the form of domain (soliton) walls. In contrast to the purely one-dimensional results[1–3] this structure corresponds in the quasi-one-dimensional case to a new thermodynamically stable phase in addition to the usual possible phases (metal, insulator). Although the only case investigated theoretically to date is that close to commensurate (1:2), there are arguments in favor of the assumption that a domain phase can exist also in incommensurate quasi-one-dimensional semiconductors. As for the purely one-dimensional result, as applied to polyacetylene $(CH)_x$ they point to the correct direction in the treatment of the experimental facts.[6] Many unanswered questions, however, still remain, particularly that of the role of the "three-dimensionality" of the electron spectrum. We consider below, just as in Refs. 4 and 5, the problem with a weakly three-dimensional electron dispersion and expect therefore a domain (soliton) superstructure to be feasible as a phase in thermodynamic equilibrium. We repeat once more that for mathematical reasons we investigate hereafter only the commensurate case. The observations already made, however, point to the existence of an analogous domain superstructure in an incommensurate charge-density wave.[7] The physical applications of our results will be discussed at the end of the article.

Our primary purpose is to study the possible physical manifestations of the domain superstructure that appears in quasi-one-dimensional semiconductors. Principal attention will be paid below to transport phenomena. We investigate in detail the features of the behavior of the conductivity of the new phase in a constant electric field (both longitudinal $\sigma_\parallel$ and transverse $\sigma_\perp$.) At low temperature we find a jumplike behavior of the conductivity anisotropy parameter $\alpha = \sigma_\perp/\sigma_\parallel$ following a (pressure) transition into a new phase, as described qualitatively in Ref. 8, and discuss also the dragging of the investigated domain superstructure by the electric field.

I. THE MODEL

We use in all the calculations that follow the previously introduced[5,9,10] simplified physical model. We assume thus that in the metallic state the electron spectrum is characterized by almost flat Fermi surfaces near $\pm p_F$, curved as a result of the finite value of the tunnel overlap integral on neighboring chains:

$$\varepsilon_{1,2}(\mathbf{p}) = \pm v_F(p_\parallel \mp p_F) - t(\mathbf{p}_\perp), \quad \int d\mathbf{p}_\perp t(\mathbf{p}_\perp) = 0, \tag{1}$$

where the form of the function $t(\mathbf{p}_\perp) = tf(\mathbf{p}_\perp)$ is not specified, and $t = \max|t(\mathbf{p}_\perp)|$. In other words, this means that we assume the presence besides the one-dimensional electron motion along the chains that make up the quasi-one-dimensional conductor, of a small but finite probability of electron hopping from one chain to another ($t \ll E_F$, where E_F is the Fermi energy).

As for the other lattice properties, we assume them to be essentially three-dimensional, i.e., we assume that in the initial phonon spectrum

$$\omega_0^2(\mathbf{k}) = \omega_0^2(2p_F, 0) + \Delta\omega_0^2(2p_F, \mathbf{k}_\perp)$$

the dispersion is not small $\Delta\omega_0^2 \sim \omega_0^2$. It is clear further that at low temperatures T and at a sufficiently small three-dimensionality of the electron spectrum t the conductor considered should be in the Peierls dielectric state. The three-dimensionality of the phonon spectrum ensures in this case, according to Ref. 11, smallness of the fluctuations and the possibility of neglecting specific one-dimensional effects outside the vicinity of the phase transition,

$$|\Delta T/T_c| > g^4\omega_0^2/\Delta\omega_0^2 \ll 1.$$

The results of Refs. 4 and 5 show, however, that the metallic and dielectric phases are not the only ones possible in the model considered here. At $T = 0$, in particular, a (pressure) phase transition is possible from the dielectric to the domain

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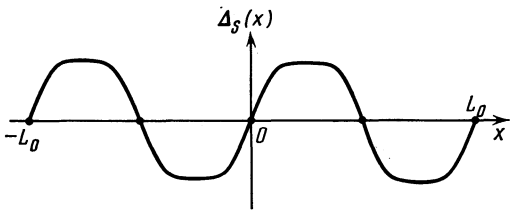

FIG. 1. Dependence of a soliton structure $\Delta_S(x)$ on the coordinate x along the chains of a quasi-one-dimensional conductor.

phase. Let us dwell here briefly on the main properties of the latter, the more so since this will be needed subsequently.

In contrast to a Peierls dielectric, the lattice deformation in the domain phase is inhomogeneous

$$D(r) \propto \Delta_s(x)\sin(2p_F x),$$

where

$$\Delta_s(x) = (E_+ - E_-)\,\mathrm{sn}[(E_+ + E_-)(x - x_0), \quad (E_+ - E_-)/(E_+ + E_-)] \tag{2}$$

is the so-called "inhomogeneous gap" of the one-dimensional problem[3] and $E_\pm$ are the band parameters (see Fig. 2).

The spatial dependence (2) of the gap on the coordinate x along the chains of a quasi-one-dimensional conductor is in essence a periodic incommensurate structure of solitons and antisolitons (Fig. 1). We note that in the plane perpendicular to the chain the lattice is not deformed, as a result of the strong dispersion of the electron-phonon interaction constant $\sim g(0) - g(\mathbf{k}_\perp) > 0$.

As for the electron spectrum of the domain phase, in the presence of the lattice deformation (2) it can be represented as the sum

$$\varepsilon(\mathbf{p}) = E(p_\parallel) - t(\mathbf{p}_\perp), \tag{3}$$

where $E(p)_\parallel$ is the spectrum of the purely one-dimensional motion in the field of the indicated deformation[3] (Fig. 2). It is assumed next that the electron bands (3) do not contain electron-hole pockets (in other words, the lower band $E < -E_+$ lies entirely below the chemical potential μ, and the upper $E > E_+$, respectively, entirely above). The central band $-E_- < E < E_-$ should, since the number of particles is the same in the dielectric and domain phases, be on the average half-filled (Fig. 3):

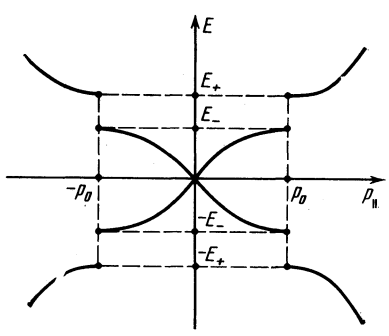

FIG. 2. Electron spectrum of one-dimensional soliton structure $\Delta_S(x)$; the wave vector is shifted by $2p_F$.

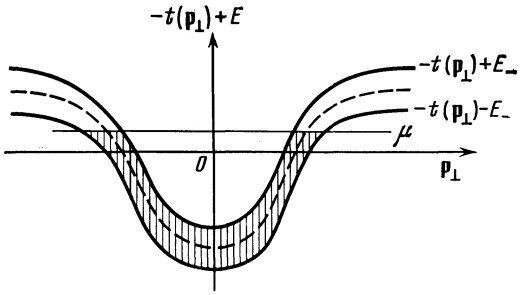

FIG. 3. Filling of the central band of the spectrum at a finite band width $2E_-$; the doubly filled states are shaded.

$$\sum_E \int_{\varepsilon(\mathbf{p})<\mu} d\mathbf{p}_\perp = \sum_E \int_{\varepsilon(\mathbf{p})>\mu} d\mathbf{p}_\perp. \tag{4}$$

We present now the main results[4,5] concerning the feasibility of a transition from the dielectric to the domain phase. In the limit of widely spaced domain walls $v_F N \ll \Delta_0$ at $T = 0$ the energy of the domain phase relative to the energy of a homogeneous dielectric was found there to be

$$\Delta W = NW_d + C_d \exp\left(-\frac{2\Delta_0}{Nv_F}\right),$$

$$W_d = \frac{2\Delta_0}{\pi} - t\int_{-t(\mathbf{p}_\perp)<\mu} f(\mathbf{p}_\perp)\frac{d\mathbf{p}_\perp}{S_\perp},$$

where $N = \Delta_0/\ln(4\Delta_0/E_-)$ is the density of such walls, Δ_0 is the gap in the dielectric, $S_\perp$ is the cross section area of the Brillouin zone, and C_d is a certain coefficient. The energy W_d of one domain wall contains, besides the positive soliton-creation energy $2\Delta_0/\pi$ (Ref. 3), also a negative integral contribution from the function $f(\mathbf{p}_\perp)$, due to the three-dimensional character of the electron motion. In fact, owing to the hopping of the electrons between the chains, the soliton energy levels make up a band in $\mathbf{p}_\perp$ and the system energy is lowered by the redistribution of the electron energies (Fig. 3).

At a certain value of the parameter $t = t^* \sim \Delta_0$ the domain-wall formation energy vanishes. For a wide class of functions $f(\mathbf{p}_\perp)$, the domain walls are exponentially repelled at $t = t^*$ ($C_d > 0$). In this case, as will hereafter be assumed, a second order phase transition takes place at $t = t^*$.

2. LONGITUDINAL CONDUCTIVITY

The question of the conductivity of commensurate quasi-one-dimensional conductors in the domain phase can be posed in simplest fashion at low temperatures ($T = 0$), where the impurity mechanism of resistivity predominates. We consider in this section the conductivity $\sigma_\parallel$ along the chains in a weak electric field, and assume that the domain superstructure is "pinned' by impurities [i.e., the pinning forces fix the origin $x_0 = \text{const}$ in (2)]. We note that at an arbitrary form of the function $t(\mathbf{p}_\perp)$ of (3) the problem is quite complicated. The physically simplest and most interesting case corresponds to the conditions at the threshold: starting from the side of the dielectric phase ($E_- = 0$) and varying the parameter t (e.g., using external pressure), we create conditions for a transition from a dielectric to the domain phase. In the

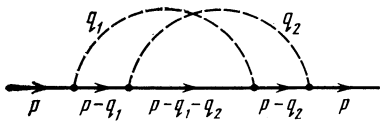

FIG. 4. "Crossing" corrections to the Green's functions for scattering by impurities.

vicinity of the transition point we have $E_- \ll \Delta_\sigma$ and the domain walls are separated by large distances L_0. A qualitatively new phenomenon appears in this region, viz., an anomalously large jump of the conductivity anisotropy parameter $\alpha = \sigma_\perp/\sigma_\parallel$. The anomalous behavior of the ratio $\sigma_\perp/\sigma_\parallel$ might be used in principle to observe experimentally the investigated phase transition.

Thus, if the superstructure is fixed, the electric resistance is due to scattering of the electrons of the central band $-E_- < E(p_\parallel) < E_-$ by impurities. The possible corrections to the electron Green's function, necessitated by this scattering, are shown in Figs. 4 and 5. We shall consider the limiting case of a very pure quasi-one-dimensional conductor, namely the case when the reciprocal scattering time satisfies the condition $1/\tau_0 \ll E_-$. This condition leaves out a large region of variation of the central electron band, $1/\tau_0 \ll E - \ll \Delta_0$, but simplifies the problem substantially. Thus, first, we can neglect the "crossing" corrections of Fig. 4 (they are of relative order $1/\tau_0 t \sim 1/\tau_0 \Delta_0$), and hence neglect all the specific one-dimensional effects connected with localization. Second, we can neglect the distortion and smearing of the band structure of Fig. 2 due to the presence of impurities, and calculate the conductivity in principal order in τ. This has reduced the problem to a determination of the damping time $\tau(E)$ of the central-band electrons, a procedure corresponding to the kinetic-equation approximation. At small $E \ll \Delta_0$ the damping time $\tau(E)$ depends little on the energy E, and we shall calculate τ below for a single domain wall. According to the diagrams of Fig. 5, the damping time is expressed in this case by the formula (the mathematical details of the derivation are given below):

$$1/\tau = -4nu_0^2 \int dx |\psi_s(x)|^4 \operatorname{Im} \left\{ \int \frac{d\mathbf{p}_\perp}{(2\pi)^2} [t(\mathbf{p}_\perp) + i\delta]^{-1} \right\},$$

where n is the impurity density and u_0 is the amplitude of the scattering by the impurities (we assume for simplicity that the scattering is isotropic, i.e., the amplitude does not depend on the wave vector p). Substituting in this expression the wave function of the soliton

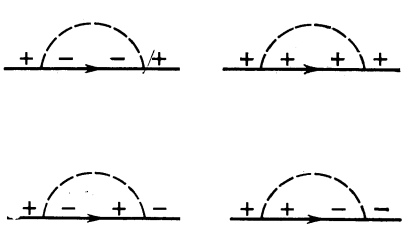

FIG. 5. Possible corrections, in scattering by impurities, to the diagonal (G^{++}, G^{--}) and off-diagonal (G^{+-}, G^{-+}) Green's functions that describe an electron subsystem in the presence of the superstructure (2).

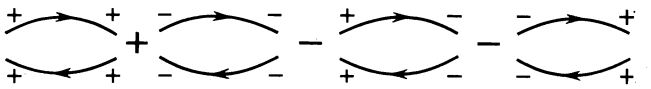

FIG. 6. Simplest diagrams for the current.

$$\psi_s(x) = (\Delta_0/2v_F)^{1/2} \operatorname{ch}^{-1}(x\Delta_0/v_F)$$

and integrating with respect to x and $\mathbf{p}_\perp$, we obtain ultimately

$$\frac{1}{\tau} = \frac{2n\Delta_0}{3v_F} u_0^2 \oint_l \frac{dl}{2\pi |\mathbf{v}_\perp(\mathbf{p}_\perp)|},$$
$$\mathbf{v}_\perp(\mathbf{p}_\perp) = -\operatorname{grad}_\perp t(\mathbf{p}_\perp). \qquad (5)$$

We have introduced in (5) the transverse velocity of the electrons on the three-dimensional Fermi surface, and the integration is along a contour l defined by the condition

$$t(\mathbf{p}_\perp) = -\mu.$$

We note that since the phase transition takes place at $t \sim \Delta_0$, the damping time of the electrons in the central band is of the same order as in an anisotropic metal: $\tau \sim \tau_0$.

We proceed now to calculate the longitudinal conductivity. Thus calls, in principle, for summation of a ladder diagram series whose first terms are shown in Figs. 6 and 7 in the coordinate representation. Since only the poles of the Green's function are significant, the calculation of these diagrams differs little mathematically from the procedure of calculating $\tau(E)$. Here and above, in the derivation of (5), we have used the fact that if there are no impurities the wave functions of the electrons in the central band are known[3] and can be written in the standard form

$$\psi_E(x) = \psi_{(+)E}(x) \exp(ip_F x) + \psi_{(-)E}(x) \exp(-ip_F x),$$
$$\psi_{(+)E}(x) = [u_E(x) + v_E(x)]/\sqrt{2}, \qquad (6)$$
$$\psi_{(-)E}(x) = [u_E(x) - v_E(x)]/\sqrt{2}.$$

We shall need also equations[12] that relate the functions u_E and v_E:

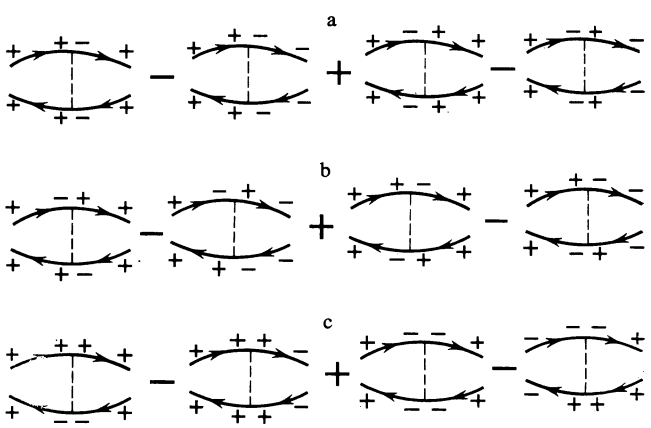

FIG. 7. First terms of the "ladder" series of diagrams corresponding to: a—scattering by $2p_F$, b—scattering with umklapp processes, c—scattering by 0.

$$v_E(x)=u_E(x)\,[-iE\Delta_s(x)\pm r^{1/2}(E)]\,[\tilde\gamma(x)-E^2]^{-1}, \qquad (6')$$

and expressions for the moduli of the wave functions

$$|v_E(x)|=\left[\frac{\gamma(x)-E^2}{2LA(E)}\right]^{1/2}, \quad |u_E(x)|=\left[\frac{\tilde\gamma(x)-E^2}{2LA(E)}\right]^{1/2}. \qquad (6'')$$

In (6′) and (6″) we have put

$$r(E)=(E_+^2-E^2)\,(E_-^2-E^2),$$

$$E_+^2+E_-^2-2\gamma(x)=\Delta_s^2(x)-\Delta_s'(x),$$

$$E_+^2+E_-^2-2\tilde\gamma(x)=\Delta_s^2(x)+\Delta_s'(x), \quad A(E)=\langle E^2-\gamma(x)\rangle,$$

where $\langle\ldots\rangle$ denotes the mean value of a function and L is the length of the system. It is obvious from the diagrams of Figs. 6 and 7 that the problem consists of simplifying the products of four wave functions of the central-band electrons, something already done when $\tau(E)$ was determined in (5) for a particular case.

We return now to diagrams 7a, b, and c. We note that they contain combinations of electron Green's functions of the type $G^{++}G^{++}-G^{+-}G^{-+}$ or $G^{--}G^{--}-G^{-+}G^{+-}$. When summing over the energies in the Green's functions only terms corresponding to the same energy need to be retained, so that the indicated combinations can be easily calculated with the aid of (6′). As a result we have

$$G^{++}(x\tilde x)\,G^{++}(\tilde x x)-G^{+-}(x\tilde x)\,G^{-+}(\tilde x x)=G^{--}(x\tilde x)$$
$$\times G^{--}(\tilde x x)-G^{-+}(x\tilde x)\,G^{+-}(\tilde x x)=\mathrm{const}\propto E_-^2,$$

i.e., they do not depend on the coordinates and are small to the extent that E_-^2 is small. Consequently, the diagrams considered are small as E_-^2 and contain no dependences on the external coordinate x. The diagrams of Fig. 6, in turn, also contain the small parameter E_-^2, i.e., they are of the same order as the diagrams of Figs. 7a, b, and c. For a correct calculation of the longitudinal conductivity we must therefore sum an infinite ladder-diagram series. It is nonetheless physically clear that this summation will lead only to replacement of the damping time τ from (5) by the transport time τ_t. Moreover, at the amplitude $u(\mathbf{p})\equiv u_0$ chosen by us for electron scattering by impurities, the diagrams of Figs. 7a, b, c vanish at any rates, and we confine ourselves below to calculation of the simplest "loops" of Fig. 6:

$$j_\parallel(x)=E_n\frac{e^2}{\pi}v_F^2\int d\tilde x\int\frac{d\mathbf{p}_\perp}{(2\pi)^2}$$
$$\times[G_R^{++}(x\tilde x,\mathbf{p}_\perp)\,G_A^{++}(\tilde x x,\mathbf{p}_\perp)$$
$$+G_R^{--}(x\tilde x,\mathbf{p}_\perp)\,G_A^{--}(\tilde x x,\mathbf{p}_\perp)-G_R^{+-}(x\tilde x,\mathbf{p}_\perp)$$
$$\times G_A^{-+}(\tilde x x,\mathbf{p}_\perp)-G_R^{-+}(x\tilde x,\mathbf{p}_\perp)\,G_A^{+-}(\tilde x x,\mathbf{p}_\perp)], \qquad (7)$$

where G_R and G_A are respectively the retarded and advanced Green's functions, and E_n is the external electric field. We now substitute in (7) the expressions for the Green's functions in terms of the wave functions:

$$j_\parallel(x)=\frac{e^2}{4\pi}v_F^2\int\frac{d\mathbf{p}_\perp}{(2\pi)^2}\int d\tilde x\sum_{-E_-<E<E_-}\frac{[u_E^*(x)v_E(x)+v_E^*(x)u_E(x)]\,[u_E^*(\tilde x)v_E(\tilde x)+v_E^*(\tilde x)u_E(\tilde x)]}{[-E+t(\mathbf{p}_\perp)+\mu+i/2\tau]\,[-E+t(\mathbf{p}_\perp)+\mu-i/2\tau]}. \qquad (7')$$

It is easy to show with the aid of (6′) that

$$u_E^*(x)v_E(x)+v_E^*(x)u_E(x)=V_E/Lv_F,$$

where $V_E=v_Fr^{1/2}(E)/A(E)$ is the longitudinal velocity of the central-band electrons, so that after integrating the expression (7′) with respect to $\mathbf{p}_\perp$ we obtain for the conductivity

$$\sigma_\parallel=\frac{e^2}{\pi}\tau\oint_l\frac{dl}{2\pi|\mathbf{v}_\perp(\mathbf{p}_\perp)|}\frac{1}{L}\sum_{-E_-<E<E_-}V_E^2, \qquad (7'')$$

which reduces, as usual, to integrating the square of the corresponding velocity projection over the Fermi surface. The state density in the central band is[3]

$$dp_\parallel/dE=A(E)/\pi v_Fr^{1/2}(E),$$

so that we obtain ultimately

$$\sigma_\parallel=2e^2\tau v_F\frac{E_-^2}{\Delta_0}\ln\frac{4\Delta_0}{E_-}\oint_l\frac{dl}{(2\pi)^2|\mathbf{v}_\perp(\mathbf{p}_\perp)|}, \qquad (8)$$

where τ is given by (5).

We note that (8) contains a very strong dependence on the domain-wall density N. According to Ref. 3, the band parameter E_- decreases exponentially as $N\to 0$:

$$E_-=4\Delta_0\exp(-\Delta_0/v_FN).$$

Thus, near the transition from the dielectric to the domain phase ($T=0$) the longitudinal conductivity is exponentially small, and if the soliton density N were increased to Δ_0/v_F this conductivity would reach the usual values $\sigma_0\sim e^2\tau_0v_FS_\perp$ of a quasi-one-dimensional metal. Substituting in (8) the expression for E_-, we get

$$\sigma_\parallel=32e^2\tau\frac{\Delta_0^2}{N}\exp\left(-\frac{2\Delta_0}{Nv_F}\right)\oint_l\frac{dl}{(2\pi)^2|\mathbf{v}_\perp(\mathbf{p}_\perp)|}. \qquad (8')$$

This drastic behavior of $\sigma_\parallel$ has a simple physical cause: at low domain-wall density N the bound soliton states decrease exponentially,

$$\psi_s(x)\sim(\Delta_0/2v_F)^{1/2}\exp(-\Delta_0x/v_F),$$

therefore the conductivity is proportional to the square of the overlap of the wave functions and decreases exponentially as $N\to 0$.

3. JUMP OF CONDUCTIVITY ANISOTROPY

It was shown in the preceding section that the longitudinal conductivity depends strongly on the domain-wall density N near the phase transition. As for the transverse conductivity $\sigma_\perp$, it contains no exponential factors, since it is determined by the conductivity inside the domain walls and

depends little on the overlap of the soliton states. In band language this means simply that the transverse component of the electron velocity on the Fermi surface

$$\mathbf{v}_\perp(\mathbf{p}_\perp) = -\operatorname{grad}_\perp t(\mathbf{p}_\perp)\,|_{t(\mathbf{p}_\perp)=-\mu}$$

depends weakly on the exponential band parameter E_-.

Thus, to find $\sigma_\perp$ it suffices to know the value of the total current $I_\perp$ inside an individual domain wall and then multiply it by the density of such walls. We note that at the scattering amplitude chosen by us, which does not depend on $\mathbf{p}_\perp$, there is no need for summing a ladder diagram, and the density of the transverse current is given by

$$j_\perp(x) = E_n \frac{e^2}{2\pi} \int d\tilde{x} \int \frac{d\mathbf{p}_\perp}{(2\pi)^2} v_n^2(\mathbf{p}_\perp) G_R^S(x\tilde{x}, \mathbf{p}_\perp) \times G_A^S(\tilde{x}x, \mathbf{p}_\perp), \tag{9}$$

where v_n is the projection of the electron velocity on the external field E_n. Rewriting the Green's function $G^S_{R(A)}(x\tilde{x}, \mathbf{p}_\perp)$ of a single soliton in terms of its wave function $\psi_S(x)$ and integrating with respect to $\mathbf{p}_\perp$ and $\tilde{x}$, we obtain

$$j_\perp(x) = E_n \frac{e^2}{2\pi} \tau |\psi_S(x)|^2 \oint_l \frac{dl}{2\pi |\mathbf{v}_\perp(\mathbf{p}_\perp)|} v_n^2(\mathbf{p}_\perp). \tag{9'}$$

Next, integrating the current density (9′) with respect to x and multiplying the result by the density N of the domain walls, we obtain ultimately

$$\sigma_\perp = \frac{e^2 N}{2\pi} \tau \oint_l \frac{dl}{2\pi |\mathbf{v}_\perp(\mathbf{p}_\perp)|} v_n^2(\mathbf{p}_\perp). \tag{10}$$

It can be seen from (10) that near the phase transition we have

$$\sigma_\perp \sim N v_F \sigma_{0\perp}/\Delta_0 \sim (t/E_F)^2 \sigma_0,$$

where $\sigma_{0\perp}$ is the transverse conductivity of a quasi-one-dimensional metal. For a developed domain superstructure, when $N \sim \Delta_0/v_F$, the transverse conductivity $\sigma_\perp$ could again have the same value as in the metallic phase.

From the results (7)′ and (10) follows a certain qualitatively new phenomenon that might help observe the dielectric–domain phase transition. At low but finite temperature the dielectric phase contains only thermally activated electrons, and although both conductivities ($\sigma_\perp$ and $\sigma_\parallel$) have additional smallness, their ratio is of the usual order of magnitude:

$$\alpha_d = (\sigma_\perp/\sigma_\parallel)_d \sim (t/E_F)^2 \sim (\Delta_0/E_F)^2.$$

Assume now that the dielectric is subjected to an external action (pressure) such that at a certain value of the external parameter the condition for spontaneous production of domain walls sets in.[4] With further change of pressure, a loose periodic structure of domain walls is produced. The conductivity anisotropy in the new phase, near the transition point, is according to (8′) and (10′)

$$\alpha(N) \sim (N v_F/E_F)^2 \exp(2\Delta_0/N v_F). \tag{11}$$

A feature of Eq. (11) is that as $N \to 0$ the conductivity-anisotropy parameter $\alpha(N) \to \infty$. In other words, at the phase-transition point ($N = 0$) the conductivity anisotropy undergoes a jump from its value $\alpha_d \sim (\Delta_0/E_F)^2$ in the dielectric phase to an anomalously large value.

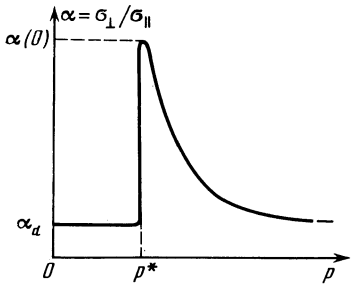

FIG. 8. Dependence of the anisotropy parameter $\alpha = \sigma_\perp/\sigma_\parallel$ on the pressure p; a phase transition takes place at the point p^* and the parameter α jumps abruptly.

Our equations are quantitatively valid if $1/\tau_0 \ll E_- \ll \Delta_0$ (we did not consider the case $E_- \lesssim 1/\tau_0$. We then obtain for the conductivity-anisotropy jump the estimate $\alpha(0) > \Delta_0^4 \tau_0^2/E_F^2 \gg 1$ for sufficiently pure quasi-one-dimensional conductors. It is physically obvious, however, that the phenomenon itself does not depend on this approximation. None of the unaccounted-for mechanisms prevents α from being large as $T, N \to 0$.

The behavior of the conductivity anisotropy as a function of an external parameter (pressure) is shown schematically in Fig. 8, and in a developed domain structure we have $\alpha \sim \alpha_d \sim (\Delta_0/E_F)^2$.

To conclude this section, we note that the phenomenon indicated is quite general and is apparently independent of any concrete model assumptions. Moreover, a similar jump of the anisotropy should be observed also in a transport phenomenon such as the Hall effect.

4. EFFECT OF AN ELECTRIC FIELD ON A DOMAIN (SOLITON) SUPERSTRUCTURE

We dwell now on the possibility of dragging of the domain structure by a constant electric field. We have assumed up to now that the superstructure is pinned by random impurities. This situation corresponds to weak electric fields. It will be shown below that an electric field, generally speaking, can drag the domain structure. We consider a case when the electric field is stronger than the pinning forces, which can therefore be neglected. In analogy with the homogeneous incommensurate case,[10] when the motion of the Fröhlich mode corresponds to a change of phase, the motion of domain superstructure corresponds to a change of the coordinate x_0 in the inhomogeneous gap (2).

It is natural to expect the force exerted by the electric field on the domain structure to be connected with the charge of the latter. We begin therefore with the question of the domain-phase charge density, given by the expression

$$\rho(x) = \sum_E \int_{\varepsilon(\mathbf{p})<\mu} \frac{d\mathbf{p}_\perp}{S_\perp} [|u_E(x)|^2 + |v_E(x)|^2], \tag{12}$$

where the functions u and v are defined by Eq. (5).

As for the central band of the electron spectrum, it shoud as already stated, be on the average half-filled [Eq. (4)]. The character of the filling of the central band at finite E_- is shown in Fig. 9. If now $E_- \to 0$, then $u(E_-) \to \mu_0$.

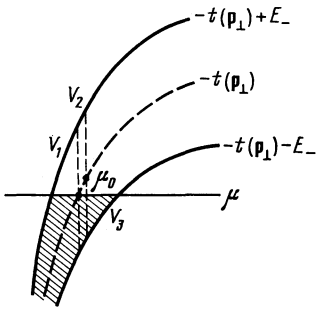

FIG. 9. Fragment of Fig. 3, the three-dimensional phase volumes V_1, V_2, and V_3 are defined in the text.

Therefore the states with $\mathbf{p}_\perp$ such that $-t(\mathbf{p}_\perp)<\mu_0$ correspond to solitons with a doubly filled level (charge $-e$), and states with $-t(p_\perp)>\mu_0$ correspond to solitons with unfilled level (charge $+e$). The condition (4) goes over as $E_-\to 0$ into

$$\int\limits_{-t(\mathbf{p}_\perp)<\mu_0} d\mathbf{p}_\perp = \int\limits_{-t(\mathbf{p}_\perp)>\mu_0} d\mathbf{p}_\perp. \tag{13}$$

Consequently the resultant charge of an isolated domain wall is equal to zero. The spatial density can then be due to overlap of the wave functions of neighboring domain walls and will be small to the extent that the parameter $E_-^4\sim\Delta_0^4\exp(-4\Delta_0/Nv_F)$ is small. Indeed, we express the charge density (12) in the form

$$\begin{aligned}\rho(x)=e\sum_{|E|<E_-}[|u_E(x)|^2+|v_E(x)|^2]\\ \times\int\limits_{-t(\mathbf{p}_\perp)<\mu_0}\frac{d\mathbf{p}_\perp}{S_\perp}+e\sum_{E<-E_+}[|u_E(x)|^2+|v_E(x)|^2]\\ +e\left(\sum_E\int\limits_{V_3}\frac{d\mathbf{p}_\perp}{S_\perp}-\sum_E\int\limits_{V_1}\frac{d\mathbf{p}_\perp}{S_\perp}-\sum_E\int\limits_{V_2}\frac{d\mathbf{p}_\perp}{S_\perp}\right)\\ \times[|u_E(x)|^2+|v_E(x)|^2],\end{aligned} \tag{14}$$

where the phase volumes V_1, V_2, and V_3 are defined as

$$\begin{aligned}V_1[0<t(\mathbf{p}_\perp)+\mu<E_-,\ t(\mathbf{p}_\perp)+\mu<E<E_-],\\ V_2[-\mu_0<t(\mathbf{p}_\perp)<-\mu,\ -E_-<E<E_-],\\ V_3[-E_-<t(\mathbf{p}_\perp)+\mu<0,\ -E_-<E<t(\mathbf{p}_\perp)+\mu].\end{aligned}$$

The sum of the first two terms in (14) is purely one-dimensional and equal to zero. It is possible also to rewrite the condition (4) in terms of the volumes V_1, V_2, and V_3:

$$\sum_E\int\limits_{V_3}d\mathbf{p}_\perp-\sum_E\int\limits_{V_1}d\mathbf{p}_\perp-\sum_E\int\limits_{V_2}d\mathbf{p}_\perp=0. \tag{15}$$

By virtue of (15) it is necessary to retain in the combination of the functions $|u_E(x)|^2+|v_E(x)|^2$ in (14) only the part that depends on the energy E. At small E we obtain

$$\rho(x)=\frac{e[\Delta_S^2(x)-\langle\Delta_S^2\rangle]}{2LA^2(0)}\times\left(\sum_E\int\limits_{V_3}\frac{d\mathbf{p}_\perp}{S_\perp}-\sum_E\int\limits_{V_1}\frac{d\mathbf{p}_\perp}{S_\perp}-\sum_E\int\limits_{V_2}\frac{d\mathbf{p}_\perp}{S_\perp}\right)E^2. \tag{16}$$

From (15) and (16) we can easily estimate the charge density $\rho(x)\sim eE_-^4/\Delta_0^3$, inasmuch the volumes in (15) are small to the extent that E_-^2 is small. For simplicity we present here a solution of (15), (16) only for the case when the function $t(\mathbf{p}_\perp)$ depends on the single variable $p_y(-p_0<p_y<p_0)$

$$\rho(x)=e[\Delta_S^2(x)-\langle\Delta_S^2\rangle]\frac{E_-^4}{16\Delta_0p_0A(0)}\frac{d^2p_y}{dt^2}\Big|_{t(p_y)=-\mu}. \tag{17}$$

It can thus be seen from (16) and (17) that at small E_- the maxima of the charge of the domain superstructure for an arbitrary form of the functions $t(\mathbf{p}_\perp)$ are always concentrated on the domain walls ($\rho(x)\to 0$ far from the walls). Their absolute value, however, is small as eE_-^4/Δ_0^3 because of the weak overlap of the soliton states. The sign of the domain-wall charge (positive or negative) depends on the concrete form of the function $t(\mathbf{p}_\perp)$. The small compensating charge will in this case be dispersed between the walls.

The appearance of a nonuniform charge density in the system calls for a separate examination of the energy contribution due to the electrostatic interaction. If $E_-\ll\Delta_0$, i.e., the conductor is near the (pressure) phase transition, the electrostatic energy $W_{el}(E_-)$ is small as E_-^8 and can be neglected even compared with the domain-wall interaction energy, which is proportional to E_-^2.

With increasing distance from the phase-transition point, the electrostatic energy increases and should, generally speaking, be taken into account when the energy functional is minimized. To estimate the Coulomb contribution it is necessary, however, to know the dielectric constant,[13] which has a strong spatial dispersion. The period of the developed domain superstructure is $L_0\sim v_F/\Delta_0$, and the dielectric constant for such values of the wave vector is close to its value in the quasi-one-dimensional metal: $\epsilon(\Delta_0/v_F)\sim 1$. As a result, at $v_F/L_0\sim\Delta_0\sim E_-$ we obtain for the ratio of the electric energy to the energy of the Peierls state the estimate

$$W_{el}/W_n\sim(E_F/\Delta_0)^2(b/a)^2,$$

where b/a is the ratio of the distances between the molecules inside the chain and between the chains themselves.

Thus, for $v_F/L_0\sim\Delta_0\sim E_-$, i.e., in a developed domain superstructure, we would have $W_{el}\gg W_n$, so that the electrostatic interaction becomes substantial even at $E_-\gtrsim E_-^*$, with $E_-^*\ll\Delta_0$. In this region the ratio

$$W_{el}/W_n\sim(E_F/\Delta_0)^2(b/a)^2(E_-^8/\varepsilon\Delta_0^8)$$

is somewhat difficult to estimate, since its dependence on the wave vector is of importance in the dielectric constant ϵ. Nonetheless, the estimates presented offer evidence that the Coulomb interaction allows the existence of a domain superstructure only in the form of relatively widely spaced walls ($v_F/L_0\ll\Delta_0$).

Returning to the question of the possibility of dragging of the domain superstructure (2) by an electric field, we note that for this purpose, generally speaking, it is necessary to calculate the force exerted directly on the superstructure by the electric field. Such a formulation of the problem, however, is too elaborate. We confine ourselves here to a different formulation, which nevertheless leads to a clear physical result.

In fact, assume that the superstructure itself moves with velocity U and ascertain whether a current is connected with this motion. To this end we write down in the general expression for the current at $T=0$ the contribution due to arbitrary small changes of the functions $\Delta_{\pm 2pF}$:

$$j_\omega(x)=2e\int d\mathbf{p}_\perp\int d\tilde{x}\int\frac{d\varepsilon}{4\pi}[G^{++}_{0\varepsilon_+}(x\tilde{x},\mathbf{p}_\perp)G^{-+}_{0\varepsilon_-}(\tilde{x}x,\mathbf{p}_\perp)$$

$$-G^{+-}_{0\varepsilon_+}(x\tilde{x},\mathbf{p}_\perp)G^{++}_{0\varepsilon_-}(\tilde{x}x,\mathbf{p}_\perp)-G^{-+}_{0\varepsilon_+}(x\tilde{x},\mathbf{p}_\perp)G^{--}_{0\varepsilon_-}(\tilde{x}x,\mathbf{p}_\perp)$$

$$+G^{--}_{0\varepsilon_+}(x\tilde{x},\mathbf{p}_\perp)G^{+-}_{0\varepsilon_-}(\tilde{x}x,\mathbf{p}_\perp)][\Delta^{(1)}_{2p_F}(\tilde{x}\omega)+\Delta^{(1)}_{-2p_F}(\tilde{x}\omega)], \quad (18)$$

where $\varepsilon_\pm=\varepsilon\pm\omega/2$, and $G_0^{\pm\pm}$ are the corresponding Feynman Green's functions in the presence of the structure (2). Substituting now in (18) the explicit expressions for the unperturbed Green's functions, we obtain

$$j_\omega(x)=2e\int d\mathbf{p}_\perp\int d\tilde{x}\int\frac{d\varepsilon}{4\pi}\sum_{E_1E_2}\frac{f_{E_1E_2}(x)\,g_{E_1E_2}(x)[\Delta^{(1)}_{2p_F}(\tilde{x}\omega)+\Delta^{(1)}_{-2p_F}(\tilde{x}\omega)]}{[\varepsilon_+-E_1+t(\mathbf{p}_\perp)+\mu+i\delta\,\mathrm{sign}\,\varepsilon_+][\varepsilon_--E_2+t(\mathbf{p}_\perp)+\mu+i\delta\,\mathrm{sign}\,\varepsilon_-]}, \quad (18')$$

where

$$f_{E_1E_2}(x)=v_{E_1}^*(x)u_{E_2}(x)+u_{E_1}^*(x)v_{E_2}(x),$$

$$g_{E_1E_2}(x)=v_{E_1}(x)u_{E_2}^*(x)-u_{E_1}(x)v_{E_2}^*(x).$$

We expand (18′) in powers of the frequency ω up to first inclusive (it can be shown that there is no zeroth order). The displacement of the superstructure as a whole is

$$\Delta^{(1)}_{2p_F}(x,\omega)+\Delta^{(1)}_{-2p_F}(x,\omega)=-d\partial\Delta_S(x)/\partial x,$$

and the frequency ω has the meaning of differentiation of the shift coordinate d with respect to time, $-i\omega d\to\partial/\partial t\, d=U$. We have therefore

$$j(x)=e\frac{iU}{4\pi}\sum_{E_1E_2}f_{E_1E_2}(x)\int d\mathbf{p}_\perp\int d\tilde{x}g_{E_1E_2}(\tilde{x})$$

$$\times\frac{\partial\Delta_S(\tilde{x})}{\partial\tilde{x}}\Big\{[-E_1+t(\mathbf{p}_\perp)+\mu+i\delta]^{-1}[-E_2+t(\mathbf{p}_\perp)+\mu-i\delta]^{-1}$$

$$+\int_{-\infty}^{0}d\varepsilon[\varepsilon-E_1+t(\mathbf{p}_\perp)+\mu-i\delta]^{-1}[\varepsilon-E_2+t(\mathbf{p}_\perp)+\mu-i\delta]^{-2}$$

$$-\int_{0}^{\infty}d\varepsilon[\varepsilon-E_1+t(\mathbf{p}_\perp)+\mu+i\delta]^{-2}[\varepsilon-E_2+t(\mathbf{p}_\perp)+\mu+i\delta]^{-1}\Big\}. \quad (18'')$$

Both summations over the energies in (18″) are over states with like quasimomenta $p_\parallel(E_2)-p_\parallel(E_1)=2mp_0$ (with account taken of the "umklapp processes"), including also over states with equal energy $E_1=E_2$. With the aid of (6′), however, it is easy to show that the matrix element

$$\int dx g_{E_1E_2}(x)\frac{\partial\Delta_S(x)}{\partial x}=\frac{1}{2}(E_1^2-E_2^2)\int dx f_{E_1E_2}(x),$$

i.e., it vanishes at $E_1=\pm E_2$. Thus, the double integral over the quasimomenta, which corresponds to the sums over the energies in (18″), does not contain any singularities. We now integrate (18″) with respect to the frequency ϵ and use the following properties of the wave functions $u_E(x)$ and $v_E(x)$ under the transformations $E\to -E$, $p_\parallel\to -p_\parallel$:

$$u_{-E(p_\parallel)}(x)=u_{E(p_\parallel)}(x),\qquad v_{-E(p_\parallel)}(x)=-v_{E(p_\parallel)}(x),$$

$$u_{E(-p_\parallel)}(x)=u^*_{E(p_\parallel)}(x),\qquad v_{E(-p_\parallel)}(x)=-v^*_{E(p_\parallel)}(x).$$

As a result we obtain for the current

$$j(x)=e\frac{iU}{4\pi}\sum_{E_1\neq E_2}f_{E_1E_2}(x)\int d\tilde{x}g_{E_1E_2}(\tilde{x})\frac{\partial\Delta_S(\tilde{x})}{\partial\tilde{x}}\int d\mathbf{p}_\perp$$

$$\times\{\theta[t(\mathbf{p}_\perp)+\mu-E_1]-\theta[t(\mathbf{p}_\perp)+\mu-E_2]$$

$$+\theta[t(\mathbf{p}_\perp)+\mu+E_1]-\theta[t(\mathbf{p}_\perp)+\mu+E_2]\}, \quad (19)$$

where $\theta(x)$ is the Heaviside step function.

We recall that the electron spectrum of our problem has no "pockets" (the chemical potential intersects only the central band). The contribution to the current differs from zero only for states such that one of the energies (for the sake of argument, E_1) lies in the central band, while the other (E_2), is outside it. From (19) it is seen next that an isolated domain wall makes no contribution to the electric current. Indeed, at $E_1=0$ we get from (19) by virtue of the condition (13)

$$j(x)\propto\int d\mathbf{p}_\perp\{2\theta[t(\mathbf{p}_\perp)+\mu_0]-1\}=0.$$

This conclusion agrees with the previous statement that an isolated domain wall has no spatial charge density. The expression for the current can be written in a form similar to the expression for the charge density (16):

$$j(x)=e\frac{iU}{4\pi}\Big(\sum_{E_1}\int_{V_3}d\mathbf{p}_\perp-\sum_{E_1}\int_{V_1}d\mathbf{p}_\perp-\sum_{E_1}\int_{V_2}d\mathbf{p}_\perp\Big)$$

$$\times\sum_{E_2}\Big[f_{E_1E_2}(x)\int d\tilde{x}g_{E_1E_2}(\tilde{x})+f_{-E_1E_2}(x)\int d\tilde{x}g_{-E_1E_2}(\tilde{x})\Big]. \quad (20)$$

Just as before, in view of the equality of the phase volumes (15), that part of the expression in the curly brackets which is independent of E_1 is cancelled out. Assuming that the indicated expression is analytic in E_1, we expand it in terms of the small parameter E_1 up to second order inclusive. We ultimately obtain the equation

$$j(x)=eU\frac{B(x)}{L\Delta_0^2}\Big(\sum_{E}\int_{V_3}d\mathbf{p}_\perp-\sum_{E}\int_{V_1}d\mathbf{p}_\perp-\sum_{E}\int_{V_2}d\mathbf{p}_\perp\Big)E^2, \quad (21)$$

where $B(x)$ is a coefficient of the order of unity [further simplification of (21) is difficult, and we present only some estimates].

It follows from (21) that, in contrast to isolated domain walls, which carry no charge, a supestructure of widely spaced domain walls can contribute to the electric current to the extent that the overlap of the soliton states is small:

$$j(x) \sim eUS_{\perp}E_{-}^{4}/\Delta_0^{3}v_F.$$

In a developed domain structure (the domain walls are not widely spaced, $E_- \sim \Delta_0$), the electric current would be of the order of

$$j(x) \sim eUS_{\perp}\Delta_0/v_F,$$

which is Δ_0/E_F times smaller than the current from a charge-density wave in the incommensurate case.[10] In other words, a small fraction Δ_0/E_F of the band electrons participates in the collective charge-transport mechanism.

Although it is physically obvious from these results that in an electric field the domain structure itself is acted upon by a force that causes it to move and participate in the conduction, the last statement was verified by us independently. The corresponding calculations are fully analogous to the preceding ones and are too lengthy to present here.

CONCLUSION

We have considered above certain physical properties of the domain (soliton) phase[4,5] of quasi-one-dimensional conductors, properties that distinguish them from the usual anisotropic metals and dielectrics. Thus, at low temperatures the conductivity anisotropy can have a narrow peak at the (pressure) transition from the dielectric into the domain phase. The value of the anisotropy parameter in the domain phase near the transition point can become quite large: $\sigma_\perp/\sigma_\parallel \ll 1$.

It was further shown that such conductors have in the domain phase an inhomogeneous charge density. In the limit of widely spaced domain walls $v_F N \ll \Delta_0$ this density is exponentially small,

$$\rho(x) \sim eE_{-}^{4}/v_F\Delta_0^{3} \sim (e\Delta_0/v_F)\exp(-4\Delta_0/Nv_F),$$

and an isolated wall has by itself no charge. The competition between the electrostatic energy and the energy of the Peierls deformation does not prevent the formation of superstructures in the form of widely spaced domain walls, but apparently hinders the formation of developed domain structures ($v_F N \sim E_- \sim \Delta_0$).

A domain superstructure can be dragged by an electric field and contribute to the electric current. In contrast to the charge-density wave in the incommensurate homogeneous case,[10] a small fraction of the band electrons participates in the indicated collective motion (or the order of $E_-^4/\Delta_0^3 E_F$ at $E_- \ll \Delta_0$ and of Δ_0/E_F in a developed domain structure). We note that owing to the spatial inhomogeneity of the charge a collective contribution of a domain superstructure to the conductivity might manifest itself as bursts of potential or current at the junctions. It was noted in Ref. 14, however, that the imperfect shape of the junctions seems to exclude the soliton mechanism as a source of generation of periodic oscillations in $NbSe_3$. It was also indicated there that these oscillations are of local origin.

In conclusion, a few words concerning incommensurate quasi-one-dimensional conductors. In this case, an analogous domain structure can be formed against the background of a sinuosidal charge-density wave. The latter is known to contribute to the collective conduction mechanism.[10] As for the domain structure, its contribution to the collective electric current is apparently zero because of the absence, in the incommensurate case, of charged solitons. The results pertaining to the jump of the conductivity anisotropy remain naturally in force in the incommensurate case.

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