# Dynamics of phase slip center of charge-density wave

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A microscopic theory is used to investigate the dynamics of the phase-slip center (PSC) in a Peierls semiconductor with nonzero energy gap $\Delta$. This center is produced when current flows in the case of a sufficiently strong deformation of a charge density wave (CDW) and constitutes a dynamic amplitude soliton. A soliton with dimension of the order of the correlation length $\xi = v/\Delta$ has a local energy level $\varepsilon = -\Delta \cos\theta$, whose position oscillates in time. A nonlinear integral equation is obtained for the total change $2\theta$ of the CDW phase on the soliton. The solution $\theta(t)$ of this equation is a function that grows stepwise with time. The voltage on the sample is directly related to $\cos\theta(t)$. The phase $\chi$ outside the PSC is described by the diffusion equation, and the quasiparticle current $j_{qp}$ is determined by the inhomogeneous deformation of the CDW ($j_{qp} \sim \chi''$). The latter is due to the screening of the CDW by quasiparticles and to band bending in the field of the inhomogeneously deformed CDW.

## 1. INTRODUCTION

One of the most interesting effects observed in inorganic quasi-one-dimensional conductors with charge density waves (CDW) is generation of narrow-band noise[1–3] (see also the reviews 4 and 5). This effect was observed in many compounds [$NbSe_3$, $TaS_3$, $K_{0,3}MoO_3$, $(TaSe_4)_2I$ and others] in which, at a certain temperature $T_P$, a Peierls transition takes place and a CDW is produced at $T < T_P$. The effect constitutes electric oscillations generated when current is passed through the sample at temperature $T < T_P$. It was observed that if the current $I$ (or the field $E$ in the sample) exceeds a certain threshold value $I_T$ (or a corresponding $E_T$) the current-voltage characteristic (IVC) of the sample becomes nonlinear, and voltage oscillations are produced in the sample and have one or several frequencies and their harmonics. The oscillation frequencies are as a rule of the order of several MHz and increase with the current. There is at present no doubt that this generation is connected with the collective conduction mechanism of these compounds—with the CDW motion. Several explanations of the generation mechanism were proposed, and some of them agree at least qualitatively with the experimental data. So far, however, no final conclusion favoring any of the proposed mechanisms can apparently be drawn.

All the proposed generation mechanism can operate either in a bulk or in a local mode. One of the simplest explanations is the so-called classical model, in which the CDW is regarded as a rigid formation acted upon by an applied field $E$, a friction force, and the force of interaction between the CDW and the lattice or the impurities. The balance equation for these forces, which determines the phase $\chi$ of the CDW, is given by[6–8]

$$\Gamma\dot{\chi} + E_T l \sin(m\chi) = El. \quad (1)$$

Here $\Gamma$ is the friction coefficient and $l$ the mean free path of the electrons. The second term in the left-hand side of (1) is due either to the interaction of a commensurate CDW with the initial lattice [in which case $m$ is an integer larger than 2 and Eq. (1) can be obtained from the microscopic theory[6]], or to the interaction of the CDW with the averaged potential of the impurities[7] (it is assumed in this case that $m = 1$, and equation is in fact phenomenological). Equation (1) jointly with the expression for the current density

$$j = \sigma_1 E + \sigma_2 \dot{\chi}/l \quad (2)$$

describes qualitatively the form of the observed IVC and explains the presence of a time-oscillating component of the CDW current.

Another possible generation mechanism is attributed not to the motion of the CDW as a whole, but to the motion of local distortions of the CDW—phase solitons or kinks.[9] In this case it is necessary to add to the left-hand side of (1) a term $-D\chi''$, in which case the equation for $\chi$ describes phase-soliton motion[10–13] that increases the conductivity of the system regardless of whether the solitons are charged[10–12] of neutral[13].[1)] The current oscillations set in when the soliton enters or leaves the sample.[9]

Other mechanisms were also proposed for the bulk generation and attributed to interaction between CDW and impurities. It was proposed in Ref. 15 that collapse of a CDW pinned by impurities takes place at $E > E_T$ as a result of quantum tunneling. In Ref. 16 the current oscillations were attributed to tunneling transitions of the electrons from one sheet of the Fermi surface to another during the time of motion of a CDW that interacts with the impurities.

Finally, local-generation mechanisms were also proposed.[17–19] Ong and Verma[19] obtained experimental evidence that the oscillations are generated not throughout the volume, but in the neighborhood of the contact. Their explanation of this phenomenon was that the inhomogeneity (e.g., of the electric field) near the contact caused the phase

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$\chi$ to increase with time, $\chi \propto Et$, at different rates in different points of the sample. The phase difference "collapse" is via formation of a phase vortex and its motion across the filaments. A local generation mechanism was proposed independently by Gor'kov,[19] who also took into account the nonuniform growth rate of $\chi$ with time. According to Gor'kov, however, the phase-difference collapse is via formation of a phase-slip center (PSC), in analogy with the situation in narrow superconducting films.[20] The growth of the gradient $\chi'$ suppresses the modulus of the order parameter $\Delta$ at a certain point to zero and changes by $2\pi$ the phase difference between the points on the left and right of the PSC. This method of generating oscillations was analyzed in detail in Refs. 19 and 21 for the case of a dirty zero-gap ($\tau\Delta \ll 1$) conductor with CDW. The absence of an energy gap has made it possible to obtain in closed form, with the aid of the microscopic theory, equations for $\Delta$ and $\chi$, and these, together with the expression for the current density, describe the behavior of the system completely. These equations were derived by Gor'kov[19] and used by him in the analysis of the dynamics of the PSC and of the current oscillations. In view of the nonlinearity and complexity of the derived equation, and analytic calculation is difficult, so that some conclusions were drawn on the basis of qualitative estimates. A computer calculation was performed in Ref. 21.

Interest attaches to a similar investigation for a more frequently occurring case, when the impurity density is not too high ($\Delta\tau \gg 1$) and the excitation spectrum of the Peierls conductor has a gap. This is precisely the purpose of the present article. It is impossible in this case to obtain for $\Delta$ and $\chi$ equations in closed form capable of describing the CDW in all of space. However, in view of the weak electric field ($El \ll \Delta$) and the short correlation length $\xi = v/\Delta$ over which $\Delta$ varies in the PSC compared with the other lengths of the problems (e.g., with the diffusion length $L_D = (D/\omega)^{1/2}$, where $\omega$ is the oscillation frequency, or with a distance $2a$ between contacts), the problem can be divided into two parts. It is possible to determine the structure of the PSC at $|x| \lesssim \xi$ (i.e., $|x| \ll L_D, a$), using directly the microscopic equation for the retarded and advanced Green's functions $g^{R(A)}$ and $f^{R(A)}$, in which $\Delta$ and $\chi$ depend on the time adibatically. The solution obtained for $\Delta$ and $\chi$ with the aid of $f^{R(A)}$ must be matched to the solution of the problem in the region $|x| \gg \xi$, where $\Delta$ and $\chi$ vary smoothly and satisfy closed-form equations that describe, in particular, the slippage, deformation, and polarization of the CDW with the screening taken into account. It was found that the PSC is in essence a dynamic amplitude soliton in which the phase $\chi$ changes by $2\theta$, and the local energy level is located at a distance $\varepsilon = -\Delta\cos\theta$ from the center of the forbidden band. Matching the solutions yields an integral equation for $\theta$ as a function of time, with a solution that is a function that has an oscillating part and grows with time. The growth rate and the oscillation frequency are proportional to the current, and the oscillation spectrum $\theta(t)$ contains many harmonics. We develop next a theory of local generation in Peierls conductors with nonzero gaps. We begin with derivation of the equations that describe the CDW outside the PSC.

## 2. QUASICLASSICAL EQUATIONS IN THE REGION OUTSIDE THE PSC

We assume the model used by us previously[22] to derive microscopic equations for the Green's functions $g$ and $g^{R(A)}$. This means that the Fermi surface of a quasi-one-dimensional metal consists of two slightly curved planes. A Peierls transition takes place in the system, a gap appears at the Fermi level, and an incommensurate CDW or a commensurate one with $m \geqslant 3$ is produced on the Fermi surface. The impurities are taken into account only to the extent that they scatter electrons. The pinning of the CDW to the impurities is neglected. Consequently, strictly speaking, at currents $I \sim I_T$ this assumption is valid only for a CDW whose pinning is due only to commensurability. Just as in Ref. 22, we use the self-consistent-field approximation. We assume also that all the quantities depend on only one coordinate $x$ along the current. To obtain the desired expressions for the current density $j$ and the charge $\rho$, and also equations for $\Delta$ and $\chi$, we must find the function $g$. We write the equation for $g$ in a quasiclassical approximation, assuming that all the functions very smoothly enough ($kv \ll \Delta$) and slowly ($\omega \ll \Delta$). For convenience we transform the matrix $\hat{g}$ by separating the phase and the generalized potential $\tilde{\Phi} = \Phi - v\chi'/2$:

$$\hat{g}(t,t') = \hat{S}(t)\hat{g}_n\hat{S}^+(t')\exp\{i\tilde{\Phi}(t-t')\},$$
$$\hat{S} = \cos(\chi(t)/2) + i\hat{\sigma}_z\sin(\chi(t)/2). \tag{3}$$

The equation for the function $\hat{g}_n$ (we omit hereafter the subscript $n$), obtained by calculating the matrix element (1), (2) from Eq. (18) of Ref. 22, takes the form

$$i\left(\hat{\sigma}_z\frac{\partial\hat{g}}{\partial t} + \frac{\partial\hat{g}}{\partial t'}\hat{\sigma}_z\right) + [\hat{\Delta},\hat{g}] + iv\frac{\partial\hat{g}}{\partial x} - iv\tilde{E}\frac{\partial\hat{g}}{\partial\varepsilon}$$
$$= \hat{\Sigma}^R\hat{g} + \hat{\Sigma}\hat{g}^A - \hat{g}^r\hat{\Sigma} - \hat{g}\hat{\Sigma}, \tag{4}$$

where $\tilde{E} = -\partial\tilde{\Phi}/\partial x$, $\hat{\Delta} = i\hat{\sigma}_y\Delta$, and $\Delta$ is the modulus of the order parameter. The matrix $\hat{\Sigma}$ describes impurity scattering:

$$\hat{\Sigma} = -(i/2)\{\nu_1\hat{\sigma}_z\hat{g}\hat{\sigma}_z - (\nu_2/2)[\hat{S}_1(t)\hat{g}\hat{S}_1(t') + \hat{S}_2(t)\hat{g}\hat{S}_2(t')]\}, \tag{5}$$

where

$$\hat{S}_1 = \hat{\sigma}_x\cos\chi + \hat{\sigma}_y\sin\chi, \qquad \hat{S}_2 = \hat{\sigma}_y\cos\chi - \hat{\sigma}_x\sin\chi,$$

$\nu_{1,2}$ are the forward- and backward-scattering frequencies. The orthogonality condition

$$\hat{g}^R\hat{g} + \hat{g}\hat{g}^A = 0 \tag{6}$$

is also useful. The functions $\hat{g}^{R(A)}$ satisfy an equation of the same form as Eq. (4), but only two terms $(\hat{\Sigma}\hat{g} - \hat{g}\hat{\Sigma})^{R(A)}$ need be retained in the right-hand side of the latter.

From Eqs. (4)–(6) we must obtain the $\hat{g}$ matrix elements with the aid of which all the measured quantities are determined. To make matters physically clearer, it is reasonable to express the matrix $\hat{g}$ in terms of a distribution function, in analogy with the procedure used for superconductors[23]:

$$\hat{g} = \hat{g}^R\hat{n} - \hat{n}\hat{g}^A, \quad \hat{n} = n_1\hat{1} + n_z\hat{\sigma}_z. \tag{7}$$

Note that at equilibrium $n_z = 0$ and $n_1 = \tanh(\bar{\varepsilon}/2T)$, i.e.,

$n_1$ is connected with the distribution functions of the quasiparticles $n$ by the relation $n_1 = 1 - 2n$. The charge and current in the system are expressed in terms of the functions $n_1$ and $n_z$, respectively. From (4) we obtain for the distribution functions $n_1$ and $n_z$ the equations

$$\left(\frac{\partial}{\partial t}+\frac{2i\Delta F_+}{G_-}+\nu_2 G_-\right) n_z=-v\frac{\partial n_1}{\partial x}+\left(v\tilde{E}-\frac{\nu_2}{2}\frac{\partial\chi}{\partial t}G_-\right)\frac{\partial n_1}{\partial\tilde{\varepsilon}}, \tag{8}$$

$$\frac{\partial n_1}{\partial t}+v\frac{\partial n_z}{\partial x}=\left(v\tilde{E}+\frac{\nu_2}{2}\frac{\partial\chi}{\partial t}\right)\frac{1}{G_-}\frac{\partial(G_- n_z)}{\partial\tilde{\varepsilon}}. \tag{9}$$

Here

$$G_-=g^R-g^A=[2\tilde{\varepsilon}/(\tilde{\varepsilon}^2-\Delta^2)^{1/2}]\,\theta(|\tilde{\varepsilon}|-\Delta),$$
$$F_+=f^R+f^A=-2i\nu_0\Delta\tilde{\varepsilon}^2/(\tilde{\varepsilon}^2-\Delta^2)^2,\quad \tilde{\varepsilon}=\varepsilon-\eta(p_\perp),\quad \nu_0=\nu_1+\nu_2/2, \tag{10}$$

$\eta(p_\perp)$ is a function that describes the Fermi-surface curvature due to the interaction between the strings. We neglect this curvature for simplicity, a procedure valid if $\eta \ll \Delta$. The terms in the right-hand side of (9) describe nonequilibrium effects that arise when current flows in the system (e.g., heating of the quasiparticles). We neglect also these effects, assuming the field not to be too strong.

Expressions for the current and charge densities can be obtained with the aid of (7) and of Eqs. (15) and (16) of Ref. 13. They take the form

$$j=\frac{\sigma_N}{l_2}\left[\int\frac{d^2p_\perp}{2S_\perp}\int_{-\varepsilon_0}^{\varepsilon_0}d\tilde{\varepsilon}\,G_- n_z+\frac{\partial\chi}{\partial t}\right], \tag{11}$$

$$\rho=\frac{\sigma_N}{vl_2}\left[\int\frac{d^2p_\perp}{2S_\perp}\int_{-\varepsilon_0}^{\varepsilon_0}d\tilde{\varepsilon}\,G_- n_1-v\frac{\partial\chi}{\partial x}\right]. \tag{12}$$

Here $\varepsilon_0$ is of the order of the Fermi energy ($\varepsilon_0 \gg \Delta, T$), $\sigma_N$ is the conductivity in the normal state (with $\Delta = 0$), $l_2 = v\tau_2 \equiv v/\nu_2$ is the mean free path, and $S_\perp$ is the area of the intersection of the Brillouin zone with a plane perpendicular to the direction of the strings. Since we neglect hereafter the dependence on $p_\perp$, we can dispense with integration with respect to $p_\perp$.

To obtain a closed set of equations it is necessary to use the self-consistency condition [see Eq. (21) of Ref. 22]. We substitute in this condition expression (7) for $\hat{g}$ and use also the form of the functions $\hat{g}^{R(A)}$ that must be found from the corresponding equations in first order in $(v\tilde{E})$. After simple transformations we obtain equations for the gap $\Delta$ and for the phase $\chi$:

$$1=\lambda\int_{-\varepsilon_0}^{\varepsilon_0}d\varepsilon\,n_1\frac{G_-}{\varepsilon}, \tag{13}$$

$$\frac{2v\tilde{E}}{\Delta^2}-\frac{v\tilde{E}}{2\Delta^2}\int d\varepsilon\,G_-\frac{\partial n_1}{\partial\varepsilon}+2\nu_0\int d\varepsilon\frac{\varepsilon^2}{(\varepsilon^2-\Delta^2)^2}n_z=0. \tag{14}$$

Equations (8)–(14) determine the behavior of the CDW for sufficiently smooth ($kv \ll \Delta$) and slow ($\omega \ll \Delta$) perturbations, in a model in which the friction of the moving CDW is due to its interaction with quasiparticles.

To illustrate the use of the derived equations, we consider first the homogeneous case of a moving CDW. In that case $n_1$ takes the equilibrium form $n_1 = \tanh(\varepsilon/2T)$. From (8) we obtain the function $n_z$ that determines the current:

$$n_z=[v\tilde{E}-(\nu_2/2)\dot{\chi}G_-]\,[2T(2i\Delta F_+/G_-+\nu_2 G_-)\,\mathrm{ch}^2(\varepsilon/2T)]^{-1}. \tag{15}$$

In this case ($\chi' = 0$) $\tilde{E} = E = -\Phi'$.

The left-hand side of (9) vanishes, and to the right-hand side, which describes the heating effects, we must add terms that describe the energy relaxation (e.g., due to scattering by phonons). In the present paper, however, we are not interested in nonequilibrium effects. With the aid of $n_z$ we can calculate the current density $j$ due to the motion of the quasiparticles and the CDW. We do note cite the calculation results, since they coincide with those of Ref. 22. The charge is zero in this case because $n_1$ is odd as a function of $\varepsilon$. From (13) we obtain for the gap the usual equation, while (14) yields for the phase the relation between $E$ and $\dot{\chi}$, calculated in Ref. 22.

The equations presented can be used also to consider another case—an immobile ($\dot{\chi} = 0$) inhomogeneous CDW in the absence of current. This situation is realized, for example, if the system contains phase solitons. It is then necessary to add to the self-consistency equation (14) for the phase a term connected with commensurability (see below and also Ref. 13). In this case the solutions of (8) and (9) are the equilibrium functions $n_z = 0$ and $n_1 = \tanh[(\varepsilon - \Psi)/2T]$, with $\Psi = \tilde{\Phi} = \Phi - v\chi'/2$, describing here the bending of the bands in the presence of a static inhomogeneous potential $\Phi$. This form of $n_1$ leads to a nonzero charge of the quasiparticles, which offsets the CDW charge [see Eq. (12)].

We turn now to the case of interest to us, when the system contains an inhomogeneous moving CDW. The function $n_1$ has again an equilibrium form, but the function $\Psi$ is no longer equal to $\Phi$ and $n_z \neq 0$. We have thus for the functions $n_1$ and $n_2$

$$n_1=\mathrm{th}\,[(\varepsilon-\Psi)/2T], \tag{16}$$

$$n_z=(v\mathscr{E}-\nu_2\dot{\chi}G_-/2)\,(\nu_2 G_-+2i\Delta F_+/G_-)^{-1}\times\{2T\,\mathrm{ch}^2\,[(\varepsilon-\Psi)/2T]\}^{-1}. \tag{17}$$

Here

$$\mathscr{E}\equiv\tilde{E}+\Psi'=(-\Phi'+\Psi'+v\chi''/2) \tag{18}$$

is the effective field that acts on the quasiparticles (the gradient of the electrochemical potential). It can be seen from (16) and (17) that the function $\Psi$ describes the deviation of the chemical potential of the quasiparticles from the center of the gap. We have assumed $\omega \ll \nu_2$ in the derivation of (17).

An expression for $\Psi$ terms of $v\chi'$ is obtained from the quasineutrality condition, i.e., from the fact that the total charge $\rho$ is zero. It may turn out that even at low temperatures ($T \ll \Delta$) the function $\Psi$ is close to $\Delta$. Coefficients such as the quasiparticle conductivity $\sigma_1$ and the friction coefficient $\Gamma$ will then not be exponentially small. Note also that the function $\Psi$ leads to suppression of the gap. Next, using (16), (17) and (11)–(14), we obtain the required equations, which are valid everywhere except in the vicinity of the PSC, where the phase $\chi$ and the modulus $\Delta$ change over distances $x \sim \xi$. For the sake of argument, we consider the low-temperature case $T \ll \Delta$, although the corresponding equations can be easily obtained analytically also in the limiting case $T \ll \Delta$. In addition, we assume that the chemical potential is not too close to $\Delta$. Thus, we calculate the coefficients in the equations for $\chi$ and $j$ subject to satisfication of the conditions

$$T \ll \Delta, \quad \Delta - |\Psi| \gg -T \ln (1-N_s), \qquad (19)$$
$$1-N_s = (2\pi\Delta/T)^{1/2} e^{-\Delta/T}.$$

Using the quasineutrality condition, to which the Poisson equation reduces in our case,[13] we obtain from (12) a relation that connects $\Psi$ with the derivative $\chi'$ of the phase:

$$2T(1-N_s) \operatorname{sh} (\Psi/T) = -v\chi'. \qquad (20)$$

From (11) we obtain an expression for the current:

$$j = \sigma_1 \mathscr{E} \operatorname{ch} (\Psi/T) + \sigma_2 \dot{\chi}/l_2, \qquad (21)$$
$$\sigma_1 = \sigma_N 4 (\nu_2/\nu_0) (T/\Delta) e^{-\Delta/T}.$$

The first term in (21) is the quasiparticle current due to the action of the effective field $\mathscr{E}$. It contains both the field-induced and the difussive quasiparticle currents. It is just the potential difference $V = \int dx \mathscr{E}$ which is measured in experiment when current flows in the case of an inhomogeneous CDW. The second term in (21) is the CDW current.

Substitution of (16) in (13) determines the change of the gap $\delta\Delta = \Delta - \Delta_0$ in the presence of the potential $\Psi$. Assuming this change to be small, we obtain under condition (19)

$$\delta\Delta/\Delta_0 = -4(T/\Delta)(1-N_s) \operatorname{sh}^2 (\Psi/2T). \qquad (22)$$

Finally, Eq. (14) for the phase $\chi$ yields

$$E - E_c \sin (m\chi) = (\dot{\chi}/l_2) (\Delta/2\pi T)^{1/2} (1-N_s) \operatorname{ch} (\Psi/T) \ln (T/\eta). \qquad (23)$$

To generalize the treatment, we have added here a term that takes commensurability effects into account (see, e.g., Ref. 13), and in the calculation of the friction coefficient we have introduced for the integral, which diverges at low energies, a low-energy cutoff $|\varepsilon| = \Delta + \eta$ (see Ref. 22). Differentiating (20) with respect to $x$ and eliminating $\Psi$ and $\widetilde{E}$ from (20), (21), and (23), we obtain the sought-for equation for the phase

$$\dot{\chi} - D_1 \chi'' + \gamma (E_c l_0) \operatorname{ch} (\Psi/T) \sin (m\chi) = (j/\sigma_N) l_2, \qquad (24)$$

where

$$D_1 = (2/\pi)^{1/2} (T/\Delta)^{3/2} l_0 v, \quad l_0 = v/\nu_0, \quad \gamma = 4(T/\Delta) e^{-\Delta/T} \ll 1.$$

In the derivation of (24) we have left out the right-hand side of (23), allowance for which leads to an exponentially small [if condition (19) is met] refinement of the coefficient of $\dot{\chi}$ in (24). The function $\Psi$, which describes the screening of the charge of the inhomogeneous CDW by the quasiparticles, is expressed in terms of $\chi'$ by relation (20). Equation (24) can be used to solve various problems in which the inhomogeneity of the CDW and hence the screening of the CDW charge are significant. We use this example to demonstrate the result of allowance for the function $\Psi$, i.e., allowance for the band bending in the case of inhomogeneous deformation of a CDW. The equation that describes an immobile phase soliton ($\dot{\chi} = 0$) in the absence of current ($j = 0$) is obtained from (24) and (20). Integrating this equation once we get

$$L_0 \tilde{\chi}' = 2[1 + (L_0^2 E_c^2/T^2) \sin^2 (\tilde{\chi}/2)]^{1/2} \sin (\tilde{\chi}/2), \qquad (25)$$

where

$$\tilde{\chi} = m\chi, \quad L_0^2 = v/[2(1-N_s) m E_c].$$

A solution that describes a single soliton (kink) is the function

$$\chi = -(2/m) \operatorname{arcctg} \{ [1 + L_0^2 (E_c/T)^2]^{1/2} \operatorname{sh} (x/L_0) \}. \qquad (26)$$

The shape and characteristic dimension of the soliton

$$L_S = L_0 [1 + L_0^2 (E_c/T)^2]^{-1/2} \qquad (27)$$

differ from those given in Ref. 13 if the radicand is not small. It follows from (27), in particular, that at low temperature $L_S$ decreases and tends to $T/E_c$, and when the temperature is raised $L_S$ has a nonmonotonic dependence on $T$ and reaches a maximum near $L_S \sim T_m/E_c$ at a temperature $T_m$ given by the equation $L_0 E_c = (\Delta T_m/2)^{1/2}$. Estimates for $TaS_3$ ($v \approx 10^8$ cm/s, $E_c \approx 1$V/cm, $\Delta \approx 800$ K) yield $T_m \approx \Delta/11 \approx 75$ K and max $L_S \approx 60\ \mu$m. If, however, no account is taken of the nonlinear dependence of $\chi'$ on the function $\Psi$, the soliton size at low temperatures can be arbitrarily large.

The dynamics of the PSC is also described by Eqs. (20) and (24). In the immediate vicinity of the PSC, however, where $\Delta$ varies over a distance $\sim \xi$, these equations no longer hold. We must therefore determine the PSC structure over distances $|x| \sim \xi$ and formulate at the location of the PSC boundary conditions for Eqs. (20) and (24).

### 3. STRUCTURE OF PSC

We turn now to the microscopic equations. We need equations only for the functions $g^{R(A)}$, since the function $g$ is expressed with the aid of (7) in terms of these functions and the distribution functions, which retain their quasiequilibrium form. The corrections to $g$, which are proportional to the external field, can be disregarded, since they are small in the vicinity of the PSC compared with gradient-containing terms. Since we consider the case of low impurity density ($\Delta\tau \gg 1$, i.e. $\xi \ll l = v\tau$), we can disregard also collisions with impurities. The equation for $\hat{g}^{R(A)}$ coincides then with Eq. (4) with zero right-hand side. We wish to find for $\hat{g}^{R(A)}$ a solution in which the phase of the order parameter is of the form $\chi(x) = \theta \operatorname{sgn} x + \alpha x$ as $|x| \to \infty$, where $\theta$ and $\alpha$ are time-dependent coefficients. Accordingly, we subject $\hat{g}^{R(A)}$ to a transformation of type (3), in which $\hat{S} = \cos(\alpha x/2) + \hat{\imath}\sigma_z \sin(\alpha x/2)$. The transformation $\Delta(x) = \widetilde{\Delta} e^{i\alpha x}$ leaves the order parameter $\widetilde{\Delta}$ complex, since the phase of $\widetilde{\Delta}$ varies from $-\theta$ to $\theta$ when $x$ changes from $-\infty$ to $+\infty$. We next find $\hat{g}^{R(A)}$ in the form [we omit the superscripts $R(A)$ for the sake of brevity]

$$\hat{g}=\hat{\sigma}_z g+\hat{\sigma}_x (f-f^+)/2+i\hat{\sigma}_y (f+f^+)/2.$$

The equation for $g, f$, and $f^+$ are of the form

$$\varepsilon f-\tilde{\Delta} g+i(v/2)f'=0,$$
$$\varepsilon f^+-\tilde{\Delta}^* g-i(v/2)f^{+\prime}=0, \quad -ff^+ + g^2=1, \tag{28}$$
$$\tilde{\Delta}^* f-\tilde{\Delta} f^+ + ivg'=0.$$

All the functions in (28) are assumed to vary slowly with time ($\omega \ll \Delta$). The equation on the right side of (28) is the normalization relation. The system (28) admits of a solution that describes an amplitude soliton with nonzero ($2\theta \neq 0$) change of the phase on it. The order parameter is of the form

$$\tilde{\Delta}=\Delta[\cos\theta+i\sin\theta\ \mathrm{th}\ (\varkappa x)], \tag{29}$$

where $\varkappa = (\Delta/v)\sin\theta$. For the Green's functions we have

$$f=\left[\tilde{\Delta}+\frac{\Delta^2\sin^2\theta}{(\varepsilon+\Delta\cos\theta)\,\mathrm{ch}^2(\varkappa x)}\right](\varepsilon^2-\Delta^2)^{-1/2},$$
$$g=\left[\varepsilon-\frac{\Delta^2\sin^2\theta}{(\varepsilon+\Delta\cos\theta)\,\mathrm{ch}^2(\varkappa x)}\right](\varepsilon^2-\Delta^2)^{-1/2}. \tag{30}$$

It is easy to verify that the functions (29) and (30) satisfy the system (28). The forms of $f$ and $g$ far from a PSC are the same as for a homogeneous CDW. Near a PSC, however, at $|x| \lesssim \xi$, their form changes. In particular, an important role is assumed by a pole at $\varepsilon = -\Delta\cos\theta$, which determines the local energy.

The coefficient $\alpha$, $\theta$, and $\Delta$ in (29) and (30) are not independent. They are related by the self-consistency condition (12). Substituting in (12)

$$\hat{g}=\mathrm{th}\,[(\varepsilon-\Psi)/2T]\,(g^R-g^A),$$

where $\hat{g}^{R(A)}$ are determined by the equations given above, we obtain two equations, one of which (for $\Delta$) coincides with (13):

$$1=\lambda\int_{-\varepsilon_0}^{\varepsilon_0} d\varepsilon\ \mathrm{th}\left(\frac{\varepsilon-\Psi}{2T}\right)\frac{G_-(\varepsilon)}{\varepsilon}, \tag{31}$$

and the other (for the phase) is

$$\int\frac{G_-(\varepsilon)\,\mathrm{th}[(\varepsilon-\Psi)/2T]}{\varepsilon(\varepsilon+\Delta\cos\theta)}d\varepsilon+2\pi\frac{\mathrm{th}[(\Delta\cos\theta+\Psi)/2T]}{\Delta|\sin\theta|}=0. \tag{32}$$

We present the values of the integrals in (31) and (32) in the limiting cases of low and high temperatures.

a) $\Delta \gg T$. We have then from (28)

$$\Delta=\Delta_0, \quad 0<\Psi<\Delta_0,$$
$$\Delta=\Delta_0(2\Psi-\Delta)^{1/2}, \quad \Delta_0/2<\Psi<\Delta_0. \tag{33}$$

We have not written out here the exponentially small gap correction of type (22), and $\Delta_0$ is the equilibrium value of the gap. It can be seen from (33) that $\Delta(\Psi)$ is a doubly valued function. We, however, are interested only in the stable branch $\Delta = \Delta_0$. From (32) we obtain the connection between $\Psi$ and $\theta$:

$$\Psi=-\Delta_0\cos\theta+T\ \mathrm{sgn}\ (\cos\theta)\ \ln F(\theta), \tag{34}$$

where

$$F(\theta)=\tilde{\theta}/(\pi-\tilde{\theta}), \quad \tilde{\theta}=\mathrm{arctg}|\mathrm{tg}\,\theta| \ \text{ for } \tilde{\theta}\gg T/\Delta,$$
$$F(\theta)=(T/2\pi\Delta)^{1/2} \ \text{ for } \tilde{\theta}\ll T/\Delta. \tag{35}$$

If Eq. (19) holds, the second term here is a small correction. The connection between $\Psi$ and the gradient $\chi' = \alpha$ of the phase is given by (20).

b) $\Delta \ll T$. Then $\Delta^2=\Delta_0^2(T)-2\Psi^2$, $\Psi=\Delta\cos\theta$.

The last result can be obtained also from the Landau-Ginzburg equation.

Equation (29) together with expressions (33) and (34) determines completely the structure of the PSC.[2)] The parameters of the PSC (e.g., the value of the gap $\Delta = \Delta_0 \cos\theta$ at $x = 0$) are found to be connected with the total phase change $2\theta$ on the PSC, which, as we shall see, increases with time and oscillates. To obtain the equation for $\theta(t)$ we must solve Eq. (24) with those boundary conditions for $\chi$ and $\chi'$ on the PSC which follow from the equations obtained in this section.

## 4. PSC DYNAMICS

The phase $\chi$ increases non-uniformly in different situations, depending on the experimental setup. To be specific, we consider one possible nonuniform increase of $\chi$. The final results of the analysis are not restricted to this formulation of the problem and can be used also in other cases. Just as in Ref. 24, where the occurrence of PSC was not taken into account, we consider CDW in a thin conductor whose diameter is small compared with the dimensions of the contacts. The latter is in turn assumed small compared with the distances between them (see Fig. 1.) A current $I$ flows through contacts 2 and 3. The phase $\chi$ averaged over the cross section is then described by Eq. (24), in which $j = (I/S)\theta(|x| - a)$, where $2a$ is the distance between contacts 2 and 3 and $S$ is the conductor cross-section area. The connection between the functions $\Psi$ and $\chi'$ is determined by (20), and the gap $\Delta$, according to (33), is constant if condition (19) is met.

We track the variation of the solution of Eqs. (20) and (24) as the current density $j$ is increased. If $j$ is less than a certain threshold value $j_{T1}$, the CDW is immobile and the stationary function $\chi(x)$ drops to zero as $|x| \to \infty$, while at $|x| > a$ the function $\chi(x)$ consists of pieces of the phase soliton (26). Expressions for $j_{T1}$ can be obtained in the limiting cases $a \ll L_S$ and $a \gg L_S$, where the length $L_S$ is defined in (27).

Consider the first case. The $\tilde{\chi}(x)$ dependence in the region $|x| > a$ is described by Eq. (25). The maximum value

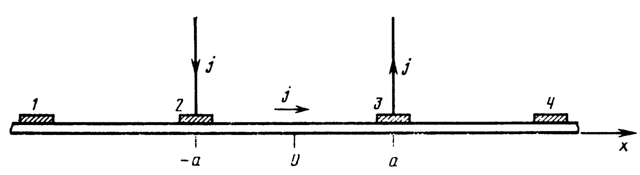


FIG. 1.

of $\tilde{\chi}'$ is $2/L_S$. If $|x|<a$ we can neglect in (24) the third term from the left ($a \ll L_S$!). Integrating this equation at $\dot{\chi}=0$, we obtain $(j/\sigma_N) l_2 a = D_1|\chi'|$. A stationary solution $\chi$ that decreases at infinity exists so long as $j$ does not exceed the threshold current $j_{T1}$ which is reached at the maximum value of $\chi'$. This yields

$$j_{T1}=2\sigma_N D_1/(a l_2 L_S). \qquad (36)$$

In the pressence of CDW deformation we have $\Psi \neq 0$, and therefore the $j(V)$ relation is not ohmic. To calculate $j(V)$ we integrate (21) from $-a$ to $a$, again neglecting $E_c \sin(m_\chi)$ compared with $\Psi'$. We get

$$j=(\sigma_1/Ta)\ \mathrm{sh}\ (V/2T), \quad V\approx\Psi(a)-\Psi(-a). \qquad (37)$$

The IVC is thus nonlinear even at $j<j_{T1}$. In the opposite limiting case $a \gg L_S$ the threshold current is $j_{T1}=\sigma_1 E_c$, and the IVC is linear: $j=\sigma_1 V/2a$.

If $j$ exceeds the threshold current $j_{T1}$, Eq. (24) has no longer a stationary solution that falls off to zero at infinity. In this case the phase will increase with time in the region $|x|<a$, and solitons will be created at $|x|>a$. In the limit as $t\to\infty$ the function $\chi(x,t)$ will approach asymptotically the solution that describes a soliton lattice at $|x|>a$.

If the current flow is large enough, $j \gg j_{T1}$, the growth dynamics of the phase $\chi$ can be described neglecting the nonlinear terms in (24), which reduces then to the diffusion equation. Assuming the phase $\chi$ and its derivative $\chi'$ to be continuous at the points $|x|=a$, we obtain for $\chi'$ at the point $x=a$, where the gradient is a maximum,

$$\chi'(a,t)=-\frac{\omega_0}{D_1^{1/2}}\left[\left(\frac{t}{\pi}\right)^{1/2}(1-e^{-a^2/D_1 t}) + \frac{2a}{(\pi D_1)^{1/2}}\int\limits_{a/(D_1 t)^{1/2}}^{\infty} e^{-y^2}dy\right], \qquad (38)$$

where $\omega_0=jl_2/\sigma_N$. The maximum value of $\chi'(a,t)$ is reached at $t\to\infty$. It is equal to $\max|\chi'(a,t)|=\omega_0 l_2/D_1$. The gradient cannot be arbitrarily large, since it is related by Eq. (20) with the potential $\Psi$, which according to (33) cannot exceed the unperturbed gap $\Delta_0$. To determine the maximum permissible value of $\chi'$ and the corresponding current $j_{T2}$ we must calculate the diffusion coefficient $D_1$ in (24) more accurately, by forgoing the second condition of (19). The calculation yields

$$j_{T2}=\left(\frac{2}{\pi}\right)^{1/2}\ln\left(\frac{e}{2}\right)\sigma_N\frac{T}{a}\left(\frac{T}{\Delta}\right)^{3/2}\frac{\nu_2}{\nu_0}. \qquad (39)$$

This quantity is usually much larger than $j_{T1}$ ($j_{T2}/j_{T1} \sim TL_S/v \gg 1$).

Consequently, if the current satisfies the inequality $j_{T1} \ll j < j_{T2}$, no PSC is formed, and the solution for $\chi'$, i.e., for the change of the CDW wave vector $Q$, is determined from the solution of the diffusion equation. This change of $Q$ diffuses into the region $|x|>a$. Let $j$ now exceed $j_{T2}$. After turning on the current $j$, the phase $\chi$ and its derivative $\chi'$ at the points $|x|=a$ will increase with time until $\chi'$ reaches the maximum allowed value. Two PSC are then produced at the points $|x|=a$ and the problem of finding $\chi(x,t)$ reduces to solving the diffusion equation with boundary conditions at the points where the PSC are located. These conditions are given by Eq. (29). They stipulate continuity of $\chi'$ and a phase jump $2\theta$ on the PSC. For example, at the point $x=a$ we have

$$\chi'(a+0)=\chi'(a-0)=\alpha, \quad \chi(a+0)-\chi(a-0)=2\theta+2\pi n, \qquad (40)$$

where $n$ is any integer,

$$\alpha=(2T/v)(1-N_s)\ \mathrm{sh}\ (\Delta\cos\theta/T).$$

Solving the diffusion equation for $\chi$ by Laplace transformation and using the boundary conditions (40) we arrive at an integral equation for $\theta(t)$:

$$2\theta(t)=\omega_0 t+\left[2T(1-N_s)\frac{D_1^{1/2}}{v}\right]\int\limits_0^t d\tau\, K(t-\tau)\,\mathrm{sh}\left(\frac{\Delta\cos\theta}{T}\right), \qquad (41)$$

where

$$K(t)=\left(\frac{D_1}{a}\right)^{1/2}\left\{1+2\sum_{n=1}^{\infty}\exp\left[-(\pi n)^2\frac{D_1 t}{a^2}\right]\right\},$$

and $\omega_0$ is defined in (38).

Equation (41) describes the PSC dynamics by determining the time dependence of the phase shift $2\theta$ on the PSC. To facilitate the analysis of this equation, it is convenient to consider the limiting cases of small and sufficiently large distances $a$ between the contacts. If $a$ satisfies the condition $a^2 \ll D_1 t_0$, where $t_0 \sim \min\{av/D_1 T, \omega_0^{-1}\}$ are the characteristic times in the $\theta(t)$ dependence, only the first term of the kernel $K(t)$ is significant. Equation (41) is then reduced upon differentiation to the form

$$2\dot{\theta}=\omega_0+\left[2T(1-N_s)\frac{D_1}{va}\right]\mathrm{sh}\left(\frac{\Delta\cos\theta}{T}\right). \qquad (42)$$

It is similar to Eq. (1), and differs only in the form of the nonlinear term. If the first term of (42) is larger than the second, the oscillation frequency is $\sim\omega_0$.

In the opposite limiting case, the sum in the kernel $K$ can be replaced by an integral. As a result, we get $K(t)=(\pi t)^{-1/2}$. Equation (41) with a kernel of this form was solved by us with a computer. The resultant $\theta(t)$ is shown in Fig. 2. It can be seen that this function takes the form of rather steep steps of height $2\pi$ (note that in this case the phase at the PSC changes by $2\theta=4\pi$). Most of the time the system is in a state in which $\cos\theta=1$, i.e., when the function $\Psi$ is close to $\Delta$. The second condition of (19), however, assumed above to be satisfied, is now violated. In this case we must take into account the second term in the right-hand side of (34) and the coordinate dependence of $\Delta$. The diffusion coefficient $D_1$, in (24) also changes:

$$\tilde{D}_1=D_1[1-2(1-N_s)\mathrm{ch}(\Psi/T)].$$

These changes merely refine the numerical coefficients in the derived relations.

Taking into account the abrupt growth of $\theta(t)$ at $\omega_0 t=2k\pi$, we can show that the function $\cos\theta(t)$ can be represented in the form

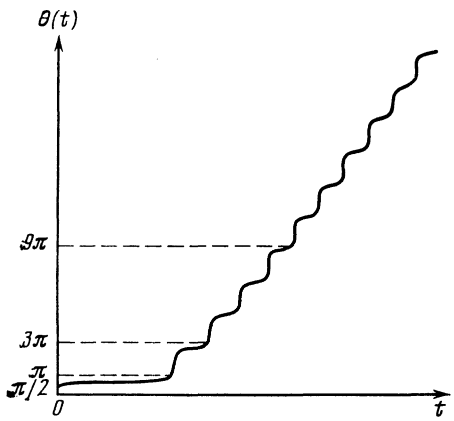


FIG. 2.

$$\cos\theta(t)=1+b(t),\quad b(t)=\sum_{k=1}^{\infty} b_k\cos(k\omega_0 t/2),\quad b_k\sim\frac{T\ln k}{\Delta k}. \tag{43}$$

The harmonics thus decrease slowly.

Let us dwell finally on the calculation of the voltages $V$ between the different points of the conductor. For $V_{14}$, for example, we have

$$V_{14}=\int_{-\infty}^{\infty}\mathscr{E}\,dx=\int_{-\infty}^{\infty}E\,dx=\frac{c_1 j}{\sigma_N}\left(\frac{\Delta}{T}\right)^{1/2}\left[a+\frac{v}{T}d(t)\right],$$

$$d(t)=\sum_{k=1}^{\infty} d_k\cos\frac{k\omega_0 t}{2},\qquad d_k\sim\frac{4\pi}{k}, \tag{44}$$

where $c_1$ is a number of the order of $\ln(T/\eta)$. The alternating component of the voltage $V_{14}$ stems from the dependence of the conductivity on the shift of the chemical pontential [see (21)]. In the calculation of $V_{14}$ we used the connection (23) between $E$ and $\dot{\chi}$, and left out the small term that describes the bulk pinning. In addition, we have assumed in the integration that the function $\Psi$ vanishes on the contacts 1 and 4 (see Fig. 1), i.e., the gradient of $\chi$ is zero at the points 1 and 4. This is correct if the $\chi'$ perturbation propagating by diffusion from the region (2,3) do not reach the points 1 and 4 during the measurement time (or during the time of the current pulse $I$). Note that the neglect of the bulk pinning in the calculation of $V_{14}$ may not be valid if the contact 1 and 4 are far enough from the region (2.3). For $V_{23}$ we have

$$V_{23}=V_{14}+2\Psi(a)=V_{14}+2\Delta\cos\theta. \tag{45}$$

The term $2\Psi(a)$ in (45) is due to the deformation of the CDW and determines the difference between $V_{23}$ and the voltage that would obtain in the homogeneous case. The function $\Psi(x,t)$ is an odd function of $x$, reaches a maximum at the points 1 and 3 and falls off as $x\to\infty$. Note that the time-varying components of the field $\mathscr{E}(x,t)$ decrease at distances $\sim(D_1/\omega_0)^{1/2}$ from the PSC.

## 5. CONCLUSION

We have developed here, under certain assumptions, a theory for the description of the phenomena in quasi-one-dimensional conductors with deformable CDW. The theory was used to analyze the local generation mechanism investigated earlier in the gapless case.[21] In the low-impurity-density case investigated here, when the energy gap is not zero, it is found that the growth of the gradient $\chi'$ of the CDW phase leads to the onset, at the point of maximum $\chi'$, of a PSC that is a dynamic amplitude soliton of size $\sim\xi=v/\Delta$. On going through the soliton, the phase $\chi$ changes by $2\theta$, and the change of $\chi'$ on the PSC is zero. The soliton can remain in an equilibrium state only if[25] $\theta=\pi/2$ (disregarding the interaction between the strings[26]). The local energy level of the dynamic soliton $\varepsilon=-\Delta\cos\theta(t)$ oscillates in time.

An important role is played also by screening effects, which shift the chemical potential from the center of the band gap. This shift, characterized by the function $\Psi$, is of great importance not only in the present problem, but also in other cases when inhomogeneous deformation of the CDW takes place. For example, allowance for $\Psi$ alters the number of quasiparticles and changes by the same token the size and shape of the phase soliton [Eq. (26)].

We have investigated a definite experimental geometry (Fig. 1), in which a PSC is formed at a point of current influx. Our results remain in force also in the case when the current $I$ flows through contacts 1–2 and 3–4. Other experimental setups are possible, in which PSC are produced and which can be described by using our present results. Differences from our case will stem from differences in the boundary conditions for the quasiclassical equations, which lead to a different $\theta(t)$ dependence and accordingly to other ac voltage amplitudes. Let us dwell briefly, for example, on another possible experimental setup. Assume a sample with a nonuniform impurity distribution, so that the threshold field $E_c$ depends on the coordinates. For example, if

$$E_c(x)=E_{c1}\theta(|x|-a)+E_{c2}\theta(a-|x|),$$

the PSC should appear at the points $x=\pm a$. It can be shown that if the condition $E_{c1}\gg E_{c2}$ is met and the mean field $\bar{E}$ is such that $E_{c2}\ll\bar{E}\ll E_{c1}$, the CDW phase $\chi$ is actually fixed at the points $x=\pm a$. There are no solutions with immobile PSC at other points. In principle, however, PSC can exist at points $|x|\neq a$, but their position will vary with time. Such a result is obtained by numerical calculation in Ref. 21, in which was analyzed a case with a phase fixed at the contact. It was found there that in the case of a phase fixed at some point, a PSC produced at another point will oscillate not only in time but also in space.

We have disregarded the influence of impurities on CDW pinning and on disruption of the long-range order. Allowance for this circumstance can change the expression for the threshold current $j_{T1}$. For large currents $j\gg j_{T1}$, in which we are mainly interested, the influence of impurities on CDW is small. Their influence is also small if the current flows through contacts 1–2 and 3–4, and the distance between contacts 2 and 3 is short. In this case no current will flow between the contacts 1 and 3, but a voltage $V=2\Delta\cos\theta$ will appear.

Despite the diligent investigations of the generation mechanism in conductors with CDW (see, e.g., the recent

Refs. 27–29), no definite conclusions can be drawn at present in favor of any of the proposed mechanisms. Nonetheless, a theoretical investigation of the local mechanism connected with the PSC is of interest since, as indicated above, it is possible to set up an experiment in which an appreciable phase gradient $\chi'$ inevitably appears, and the onset of PSC is thereby facilitated.

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[1)]It is concluded, in a recent report[14] of measurement of the conductivity of $TaS_3$ under tension, that it is just the kinks which cause the nonlinearity of the IVC.

[2)]Brazovskiĭ[25] has shown that a soliton with $\theta \neq \pi/2$ cannot exist in equilibrium, since it does not meet a condition of type (32) for a phase with $\Psi = 0$.

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