The role of Coulomb effects in the electrodynamics of a quasi-one-dimensional charge density wave

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We investigate the role of interelectron Coulomb interactions in the tunneling production of soliton-antisoliton charge carriers by a constant electric field from the condensate of a charge density wave. We show that due to the pronounced anisotropy of the permittivity in fields with $E_T < E < E_T^*$ (E_T is a one-dimensional threshold field), there is a spatial region $\xi_\perp$ of coherent production in which the Coulomb field is one-dimensional and gives a production threshold E_T. This mechanism accounts for the experimental threshold dependence of the nonlinear conductivity on the field. In fields $E \gg E_T^*$, the problem becomes three-dimensional. The size of $\xi_\perp$ is governed by the competition between transverse dispersion and Coulomb interaction.

The unusual electrodynamic properties of quasi-one-dimensional conductors in the dielectric phase have long been of scientific interest. Compounds which make a low-temperature transition to a Peierls dielectric (PD) state have been studied in particular detail. A PD is characterized by a complex order parameter $\Delta\exp(i\varphi)$, with the modulus Δ determining the gap in the one-particle excitation spectrum, and the phase describing the dynamics of a charge density wave (CDW). Widely used PD such as TaS_3, $K_{0.3}MoO_3$, $NbSe_3$, and a number of others comprise a set of one-dimensional conducting chains with an anisotropic electron spectrum $t_\parallel \gg t_\perp$, where $t_{\parallel,\perp}$ are electron integrals for a transition between adjacent nodes of the chains in the direction of one-dimensionality (along the chains) and across the chains (for example, see the review in Ref. 1).

The smallness of the transverse characteristics of a PD compared with the longitudinal characteristics have long made it possible to restrict the theoretical description of the longitudinal response of a CDW to a purely one-dimensional approximation. Roughly speaking, the role of the transverse dynamics is then reduced to maintaining long-range order in the system. More recently, however, it has been shown that interchain interaction due to the three-dimensionality of the crystal electron and phonon spectra profoundly influence the dynamics and thermodynamics of a PD (see the reviews in Refs. 2 and 3). In Ref. 4 and other works of these same authors, a three-dimensional representation is also employed in the description of CDW electrodynamics.

Nevertheless, the three-dimensionality of the problem does not simply reduce to consideration of the transverse spectral dispersion. In a system with charge-carrying excitations, it is important to determine the electric field in a self-consistent manner. In a PD, if there exist free electron (holes) with high mobility and sufficient density ρ, the electric field will be determined by the requirement of local electrical neutrality[4] $\delta\rho = 0$, as in the theory of metals. Free quasiparticles then screen CDW excitation charges. For local electrical neutrality to hold, the mean free path (or the localization length) l for free carriers must be much greater than the Debye screening length, $l \gg r_D$. In real Peierls dielectrics this condition can often be violated; there is no Debye screening, and the field E is found by solving the Poisson equation, or what is the same, by obtaining a solution which takes electron Coulomb interactions explicitly into account.

Taking the Coulomb field into account in CDW electrodynamics when there is no Debye screening is found to be of fundamental importance in studies of the nature of the threshold electric field in nonlinear CDW conductivity along the chains.[5] It is known from experiments[1] that the PD conductivity is of the form

$$\sigma(E) = \sigma_0 + \left(1 - \frac{E_T}{E}\right)\sigma_1 \exp\left[-\frac{E_0}{E - E_T}\right], \quad E > E_T, \quad (1)$$

where σ_0 is the ohmic conductivity due to free carriers, the second term in (1) is due to CDW conductivity, E is a constant and uniform external field, and the field E_T is a universal characteristic of the sample. The conductivity σ_0 depends on the temperature through the Mott relation[14]

$$\sigma_0 \sim \exp[-(T_0/T)^{1/4}],$$

so it can be shown that at low temperatures, the free carriers are strongly localized, and do not provide Debye screening. With this assumption, a mechanism has been proposed[5] for the conductivity (1), based on the idea of a CDW soliton tunneling conductivity. As is well known,[1] nonlinear current-carrying excitations, solitons (s) and antisolitons ($\bar{s}$) of phase φ, exist in a commensurate CDW. In the absence of an external electric field E at low temperatures, these are bound in a homogeneous CDW condensate into $s\bar{s}$ pairs. Through tunneling, the electric field can produce solitons and antisolitons by dissociating the pairs. If we assume, as in Ref. 5, that $s\bar{s}$ pair production occurs coherently, along the chains, i.e., $s\bar{s}$ walls are produced with macroscopic size $\xi_\perp \gg a_\perp$ ($a_\perp$ is the distance between chains), then the Coulomb field of the pairs within a cluster will be one-dimensional, and will give a production threshold E_T. The value of E_T found in this manner describes the experimental data surprisingly well, at least at low temperatures. Furthermore, the evidence

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of both indirect experiments[1] and direct observation of significant broadening of the x ray peak for the transverse component $q_\perp$ of the wave vector in fields $E > E_T$ [Ref. 6] confirms the cluster nature of E_T. It has been shown experimentally[6] that for $E > E_T$, there is a transverse macroscopic length $\sim 10^2$ Å which can be identified with $\xi_\perp$.

Nevertheless, the approach taken in Ref. 5 is unsatisfactory from a theoretical standpoint, since the hypothesized transverse coherence of the soliton walls has not been substantiated. In the present paper, we attempt to put the cluster model on a firm foundation. The macroscopic transverse dimension $\xi_\perp$ arises as a result of competition between the dispersion of the PD spectrum and interelectron Coulomb interaction. It turns out that for $s\bar{s}$ pair production by an external field, there is always a region of one-dimensional Coulomb interaction $\xi_\perp$ when $E > E_T$. We have also found the dependence of $\xi_\perp$ on the field and the system parameters.

The physical reason for cluster production is apparent. Transverse dispersion basically tends to establish states with $\varphi = \text{const}$, while to minimize the Coulomb energy, it is advantageous to alternate changes in chains; the result is a $\xi_\perp$ region.

Although the present work has been carried out in order to clarify the experimental function (1), an important element has been left out, namely the presence of impurities, which are well known[7,8] to destroy CDW coherence. We shall assume that $\xi_\perp$ is less than the correlation length of the impurity potential.

STATEMENT OF THE PROBLEM: CDW LAGRANGIAN IN THE PRESENCE OF COULOMB INTERACTION

The starting point for the microscopic theory is the Hamiltonian of a quasi-one-dimensional PD, written in the nodal approximation:

$$H = \frac{1}{2}\sum_{n,j,a} K(\mathbf{r}|\mathbf{r}+\mathbf{a})\,(\mathbf{u}_\mathbf{r}-\mathbf{u}_{\mathbf{r}+\mathbf{a}})^2 + \frac{M_i}{2}\sum_{n,j}\dot{\mathbf{u}}_\mathbf{r}^2$$
$$+ \sum_{n,j,s} t_{n,n+1}(c^+_{njs}c_{n+1js} + \text{c. c.}) + t_\perp \sum_{n,j,a_\perp,s} c^+_{njs}c_{nj+\mathbf{a}_\perp s}$$
$$+ e^2 \sum_{n,j,n',j',s} \frac{\hat{n}_e(\mathbf{r})\hat{n}_e(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} - ee^* \sum_{n,j,n',j',s} \frac{\hat{n}_e(\mathbf{r})\,\mathrm{div}\,\mathbf{u}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$
$$+ e^{*2} \sum_{n,j,n',j'} \frac{\mathrm{div}\,\mathbf{u}(\mathbf{r})\,\mathrm{div}\,\mathbf{u}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} = H_F + H_Q. \qquad (2)$$

Here the first four terms are essentially the usual Fröhlich Hamiltonian H_F, and the last three are combined into H_Q, and correspond to the Coulomb interaction between electrons alone, between electrons and ions, and between ions alone.

Our notation is as follows: K is the elasticity matrix of the lattice, M_i is an ion mass, $\mathbf{u}_\mathbf{r}$ is the displacement of a lattice site, $\mathbf{r} = (na, ja_\perp)$, n is a site index along the chain, j is the chain index, a is the interatomic distance along the chain, $a_\perp$ is the distance between chains, $t_{n,n+1}$ is the electron jump integral between neighboring sites along the chain, $t_\perp$ is the electron jump integral between chains, $c_\mathbf{r}$ is the electron operator, e is the charge on the electron, e^* is the ion charge, $\hat{n}_e = c_s + c_s$ is the electron density operator, and s is the spin index.

In the Peierls phase, the lattice displacement is

$$\mathbf{u}(\mathbf{r}) = u_0(\mathbf{r})\cos[\mathbf{Q}\mathbf{r}+\varphi(\mathbf{r})]\mathbf{x}, \qquad (3)$$

where $\mathbf{Q}$ is the CDW vector,[3]

$$\mathbf{Q} = (2k_F, \mathbf{Q}_\perp), \quad |\mathbf{Q}_\perp| \ll 2k_F.$$

Taking the standard approach,[5] we expand the integral of longitudinal electron jumps $t_{n,n+1}$ in a power series in the displacements

$$t_{n,n+1} = \sum_{m=0}^{\infty} t_m (u_n - u_{n+1})^m, \qquad (4)$$

and we represent the electron operators c_{rs} in the form

$$c_{rs} = 2^{-1/2}\{W_s(\mathbf{Q}_\perp, \mathbf{r})\exp\{ik_F na\} + V_s(\mathbf{Q}_\perp, \mathbf{r})\exp\{-ik_F an\}\}, \qquad (5)$$

where W and V are smooth functions with a scale length k_F^{-1}. Substituting (3), (4), and (5) into (2) and averaging over rapid oscillations with the period of the lattice, we obtain the Hamiltonian for a continuum PD model in which the only parameter variations are those which are large relative to $\mathbf{a}$.

With $|\mathbf{Q}_\perp| \ll \nabla_\perp$, we have the Hamiltonian density (the details of the derivation of the one-dimensional part can be found in Ref. 5)

$$n_f^{-1}h = \frac{\Delta^2}{2g^2}(1+\eta a_\perp^2(\nabla_\perp\varphi)^2) + \frac{\dot{\Delta}^2+\Delta^2\dot{\varphi}^2}{2g^2\omega_Q^2} - \hbar v_F \bar{\Psi}_s\sigma_1\partial_x\Psi_s$$
$$+ \Delta\bar{\Psi}_s\exp(-i\sigma_3\varphi)\Psi_s + \mu\Delta\bar{\Psi}_s\exp(i\sigma_3\theta)\Psi_s + \hbar v_\perp\bar{\Psi}_s\sigma_2\nabla_\perp\Psi_s$$
$$+ e^2 n_f \int d\mathbf{r}' \frac{(\bar{\Psi}_s\sigma_2\Psi_s)_\mathbf{r}(\bar{\Psi}_s\sigma_2\Psi_s)_{\mathbf{r}'}}{|\mathbf{r}-\mathbf{r}'|}. \qquad (6)$$

Here

$$\hbar v_F = t_0, \quad \Delta = 2t_1u_0/a, \quad g^{-2} = K_\parallel a\sin^2(k_Fa)/16t_1^2,$$
$$\omega_Q^2 = K_\parallel/2M_i, \quad \Psi_s = \begin{pmatrix} W_s \\ V_s \end{pmatrix}, \quad \bar{\Psi}_s = \Psi_s^+\sigma_2,$$

σ_i are the Pauli spin matrices, $\mu \sim (\Delta/\varepsilon_F)^{M-2} \ll 1$, $M = \pi/k_Fa$ is the commensurability index of the PD (M is an integer, with $M > 2$), $\hbar v_\perp t_\perp a_\perp/a$, $\eta = K_\perp/K_\parallel$ is the phonon anisotropy constant,

$$K_\parallel = K(x, \mathbf{j}|x+a, \mathbf{j}), \quad K_\perp = K(x, \mathbf{j}|x, \mathbf{j}+\mathbf{a}_\perp), \quad \varphi = \varphi + 2\mathbf{Q}_\perp\mathbf{j},$$
$$\theta = (M-1)\varphi - {}^1/_2\pi M + Mk_Fa,$$

and n_f is the density of the chains.

The one-dimensional part of η, i.e., Eq. (6) with $\eta = v_\perp = 0$, is naturally the same, in the absence of the Coulomb term, as the usual form for the one-dimensional continuum model.[2,5]

Note that of the three "bare" Coulomb terms in (2), only the electron-electron interaction enters into the continuum Hamiltonian. It is in fact easy to show that for the Peierls displacement (3),

$$ee^{*}\sum_{\mathbf{r}'}\frac{n_e(\mathbf{r})\operatorname{div}\mathbf{u}(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}\approx\frac{ee^{*}}{a\varepsilon_F}\Delta\bar{\Psi}_s\exp(-i\sigma_3\varphi)\Psi_s, \quad (7)$$

$$e^{*2}\sum_{\mathbf{r}'}\frac{\operatorname{div}\mathbf{u}(\mathbf{r})\operatorname{div}\mathbf{u}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\approx\frac{e^{*2}}{a\varepsilon_F}\Delta^2, \quad (8)$$

i.e., these terms simply give rise to a renormalization of the electron lattice coupling constant g, which is perfectly natural for a description within the context of the Fröhlich model.

In what follows, it will be most convenient to make use not of the Hamiltonian h, but of the corresponding Lagrangian

$$\mathcal{L}=\hbar i\bar{\Psi}_s\sigma_2(\partial_t-ieEx/\hbar)\Psi_s-h, \quad (9)$$

where E is a constant and uniform external electric field.

Starting now with the microscopic Lagrangian (9), we derive an effective PD Lagrangian which contains only the order parameter Δ and φ as components. As is well known (see Ref. 5, for example), the effective Lagrangian may be expressed in terms of the PD partition function, expressed as the functional

$$Z=\int D\Delta D\varphi D\bar{\Psi}_s D\Psi_s\exp\left(\int d\mathbf{r}\,d\tau\,\mathcal{L}\right)$$
$$=\int D\Delta D\varphi\exp\left(\int d\mathbf{r}\,d\tau\,\mathcal{L}_{eff}\right), \quad (10)$$

where $\tau=-it$ is imaginary time ($0\leqslant\tau\leqslant\beta$), and β is the reciprocal of the temperature.

For fermion fields $\bar{\Psi}$ and Ψ, the functional integral in the form (6) cannot be calculated, so we make use of the following convenient representation for the Coulomb term[9]:

$$\exp\left\{-e^2n_f^2\int d\mathbf{r}\,d\mathbf{r}'\,d\tau\frac{(\bar{\Psi}\sigma_2\Psi)_{\mathbf{r}}(\bar{\Psi}\sigma_2\Psi)_{\mathbf{r}'}}{|\mathbf{r}-\mathbf{r}'|}\right\}$$
$$=\int D\chi\exp\left\{-\int d\mathbf{r}\,d\tau\left[\frac{1}{8\pi}(\nabla\chi)^2+ien_f\chi\bar{\Psi}\sigma_2\Psi\right]\right\}. \quad (11)$$

Equation (11) uses the relation

$$\Delta_{\mathbf{r}}\frac{1}{|\mathbf{r}-\mathbf{r}'|}=-4\pi\delta(\mathbf{r}-\mathbf{r}'), \quad (12)$$

where $\Delta_{\mathbf{r}}$ is the Laplacian operator.

After substitution of (11) into (10), the fermion functional is calculated easily, since it becomes Gaussian, and we have

$$Z=\int D\Delta D\varphi D\chi\exp\left(\int d\mathbf{r}\,d\tau\mathcal{L}_{lat}\right)$$
$$\times\exp\left[-\int d\mathbf{r}\,d\tau\frac{1}{8\pi}(\nabla\chi)^2\right]\int D\bar{\Psi}_s D\Psi_s$$
$$\times\exp\left(\int d\mathbf{r}\,d\tau\,\mathcal{L}_{el}\right), \quad (13)$$

where

$$\mathcal{L}_{lat}=-n_f\left\{\frac{\Delta^2}{2g^2}[1+\eta a_\perp^2(\nabla_\perp\varphi)^2]+\frac{\dot{\Delta}^2+\Delta^2\dot{\varphi}^2}{2g^2\omega_Q^2}\right\}, \quad (14)$$

$$\mathcal{L}_{el}=n_f\bar{\Psi}_s\left\{-\hbar\sigma_2\left(\partial_\tau-\frac{e}{\hbar}Ex-ie\chi\right)+\hbar v_F\sigma_1\partial_x-\Delta\exp(-i\sigma_3\varphi)\right.$$
$$\left.-\mu\Delta\exp(i\sigma_3\theta)-\hbar v_\perp\sigma_2\nabla_\perp\right\}\Psi_s. \quad (15)$$

In doing the fermion integration, it is convenient to make the following change of variables in the functional integral, separating out the so-called homogeneous chiral anomaly[5,10]:

$$\Psi\to\exp\left(i\frac{\sigma_3\varphi}{2}\right)\exp\left(i\frac{v_F}{2}\int d\tau\varphi'\right)\tilde{\Psi}, \quad (16)$$
$$\bar{\Psi}\to\tilde{\bar{\Psi}}\exp\left(i\frac{\sigma_3\varphi}{2}\right)\exp\left(-i\frac{v_F}{2}\int d\tau\varphi'\right).$$

As is well known,[5,10] the Jacobian associated with the transformation (16) is

$$J=\exp\left(-n_f\int d\mathbf{r}\,d\varphi\left\{\frac{\hbar}{4\pi v_F}[\dot{\varphi}^2+v_F^2(\varphi')^2]\right.\right.$$
$$\left.\left.-\frac{e}{\pi}E\varphi-i\frac{e}{\pi}\chi\varphi'\right\}\right). \quad (17)$$

Thus, we must calculate the following fermion determinant:

$$\int D\tilde{\bar{\Psi}}_s D\tilde{\Psi}_s\exp\left\{n_f\tilde{\bar{\Psi}}_s\left[-\hbar\sigma_2\left(\partial_\tau-\frac{e}{\hbar}Ex-ie\chi\right)\right.\right.$$
$$+\hbar v_F\sigma_1\partial_x-\Delta-\mu\Delta\exp(i\sigma_3M\varphi)$$
$$\left.\left.-\hbar v_\perp\sigma_2\nabla_\perp+\frac{v_\perp}{2v_F}(\nabla_\perp\varphi)\right]\Psi_s\right\}$$
$$=\exp\operatorname{Sp}\ln\hat{L}, \quad (18)$$

where $\hat{L}$ is the operator in square brackets,

$$\operatorname{Sp}\hat{A}=\frac{2n_f}{\hbar}\operatorname{Tr}\int d\mathbf{r}\,d\tau\langle\mathbf{r}\tau|\hat{A}|\mathbf{r}\tau\rangle, \quad (19)$$

and Tr denotes summation over the matrix indices.

As usual,[11] in imaginary time we make the substitutions $E\to iH$ and $\chi\to i\chi$. We also perform a canonical transformation on the operator $\hat{L}$:

$$\hat{L}\to\exp\left[-i\frac{e\tau}{\hbar}(\chi+Hx)\right]\hat{L}\exp\left[i\frac{e\tau}{\hbar}(\chi+Hx)\right], \quad (20)$$

following which it turns out to be convenient to calculate the quantity

$$\operatorname{Sp}\ln(\hat{K}_0+\hat{K}_1)=2\operatorname{Sp}\ln\hat{L}, \quad (21)$$

where

$$\hat{K}_0+\hat{K}_1=\hat{L}\sigma_3\hat{L}\sigma_3 \quad (22)$$

and

$$\hat{K}_0=-\hbar^2\partial_\tau^2-v_F^2\hbar^2\left(\partial_x-\frac{eH\tau}{\hbar}-i\frac{e\chi'\tau}{\hbar}\right)^2$$
$$+\Delta^2+e\hbar v_F\sigma_3(H+i\chi'), \quad (23)$$

while

$$\hat{K}_1=2\Delta^2\mu\exp(i\sigma_3M\varphi)-\frac{\hbar^2v_\perp^2}{4}(\nabla_\perp\varphi)^2$$
$$-\hbar v_\perp v_F(\nabla_\perp\varphi)\partial_x+\hbar ev_\perp(\nabla_\perp\chi)-\hbar^2v_\perp^2\nabla_\perp^2. \quad (24)$$

The operator was split into $\hat{K}_0$ and $\hat{K}_1$ for the same reasons as in Ref. 5. The operator $\hat{K}_0$ accounts for the purely "one-dimensional" contribution to the electron energy, and depends solely on the modulus Δ of the order parameter. The entire phase-dependence of the energy is contained in $\hat{K}_1$. In calculating $\hat{K}_0$ and $\hat{K}_1$, we have made use of the condition $\Delta \gg \hbar v_\perp \nabla_\perp$, according to which the energy associated with Δ at $T=0$ is independent of the transverse coordinates. Strictly speaking, the latter condition only holds when $\chi'/\chi \ll \xi_0^{-1}$ ($\xi_0 = \hbar v_F/\Delta_0$ is the longitudinal coherence length of the PD, and Δ_0 is the field-free value of Δ at $T=0$).

Following the development in Ref. 5, we represent the partition function Z in the form

$$Z = \int D\chi \exp\left[\int d\mathbf{r}\, d\tau \frac{1}{8\pi}(\nabla\chi)^2 \right]$$

$$\times \int D\Delta \exp\left\{ -\int d\mathbf{r}\, d\tau\, n_f \left[\frac{\Delta^2}{2g^2} + \frac{\dot{\Delta}^2}{2g^2\omega_Q^2} \right] + \frac{1}{2} \operatorname{Sp} \ln \hat{K}_0 \right\}$$

$$\times \int D\varphi \exp\left\{ -\int d\mathbf{r}\, d\tau\, n_f \left[\eta \frac{\Delta^2}{2g^2} a_\perp^2 (\nabla_\perp \varphi)^2 + \frac{\Delta^2 \dot{\varphi}^2}{2g^2\omega_Q^2} \right.\right.$$

$$\left. - \frac{\hbar}{4\pi v_F}(\dot{\varphi}^2 + v_F^2(\varphi')^2) - i\frac{e}{\pi} H\varphi + \frac{e}{\pi}\chi'\varphi \right]$$

$$\left. + \frac{1}{2} \operatorname{Sp} \ln (1 + \hat{K}_0^{-1}\hat{K}_1) \right\}. \qquad (25)$$

By making use of the PD adiabaticity parameter[2] $g\omega_Q(\hbar v_F)^{-1/2} \ll \Delta$, we can, in Eq. (25), firstly neglect the time derivative in the chiral anomaly compared with the term $\Delta^2\dot{\varphi}^2/g^2\omega_Q^2$, and secondly, calculate the inner integral over $D\Delta$ by the method of steepest descent.[5,11] We obtain

$$\int D\Delta \exp\left(-\int d\mathbf{r}\, d\tau \frac{n_f \Delta^2}{2g^2} + \frac{1}{2} \operatorname{Sp} \ln \hat{K}_0 \right)$$

$$\approx \exp\left(\int d\mathbf{r}\, d\tau \left[\frac{n_f \Delta_0^2}{2\pi\hbar v_F} - \frac{\varepsilon_\Delta}{8\pi}(H + i\chi')^2 \right] \right), \qquad (26)$$

where $\varepsilon_\Delta = 4e^2 n_f \xi_0/3\Delta_0$ is the permittivity of the framework. The term containing ε_Δ was derived for $T=0$ assuming that $\chi'/\chi \ll \xi_0^{-1}$ and $|H|, |\chi'| \ll E_C$, where $E_C \sim \Delta_0^2/e\hbar v_F$ is the field which destroys the Peierls phase.[11] The latter approximation is physically self-evident, as otherwise the PD does not exist. Further calculations verify the smallness of the longitudinal gradients of χ.

In calculating $\operatorname{Sp} \ln(1 + \hat{K}_0^{-1}\hat{K}_1)$, we make use of the Green's function method for a PD in a constant electric field developed in Ref. 12:

$$\operatorname{Sp} \ln(1 + \hat{K}_0^{-1}\hat{K}_1) \approx \operatorname{Sp} \hat{K}_0^{-1}\hat{K}_1 - {}^1\!/_2 \operatorname{Sp} \hat{K}_0^{-1}\hat{K}_1\hat{K}_0^{-1}\hat{K}_1 \qquad (27)$$

and $\langle \mathbf{r}\tau | \hat{K}_0^{-1} | \mathbf{r}'\tau' \rangle = \frac{1}{2\pi}\left(\frac{e\tilde{H}}{\pi}\right)^{1/2} \int dp \exp[ip(x-x')]$

$$\times \sum_{n=0}^{\infty} \frac{1}{n!} D_n\left[(2e\tilde{H})^{1/2}\left(\tau - \frac{p}{e\tilde{H}} \right) \right]$$

$$\times D_n\left[(2e\tilde{H})^{1/2}\left(\tau' - \frac{p}{e\tilde{H}} \right) \right] \begin{pmatrix} \lambda_1^{-1} & 0 \\ 0 & \lambda_{-1}^{-1} \end{pmatrix}, \qquad (28)$$

$\lambda_{\pm 1} = (2n + 1 + \nu)e\tilde{H}$, $\nu = \pm 1$, $\hbar = v_F = 1$, $\tilde{H} = H + i\chi'$, and D_n is a parabolic cylinder function.

Omitting the calculations for (27) using (28), we immediately give the result for the effective PD Lagrangian (10), which has already been given in terms of real time:

$$\exp\left(i \int d\mathbf{r}\, dt\, \mathscr{L}_{eff} \right)$$

$$= \int D\chi \exp\left\{ i \int d\mathbf{r}\, dt \left[\frac{\varepsilon_\Delta}{8\pi}(\chi')^2 + \frac{\varepsilon_\perp}{8\pi}(\nabla_\perp\chi)^2 \right.\right.$$

$$\left. - i\frac{e}{\pi} n_f \chi'\varphi \right] \right\} \exp\left\{ i \int d\mathbf{r}\, dt \left[\frac{\varepsilon_\Delta E^2}{8\pi} + \frac{n_f}{\pi\hbar v_F}\left(\frac{\Delta^2}{2} \right.\right.\right.$$

$$+ \frac{\Delta^2\dot{\varphi}^2}{\lambda\omega_Q^2} - \frac{\hbar^2 v_F^2}{4}(\varphi')^2$$

$$\left.\left.\left. - \frac{\hbar^2 \tilde{v}_\perp^2}{4}(\nabla_\perp\varphi)^2 - eE\hbar v_F\varphi + \frac{2\Delta^2\mu}{\lambda}\cos M\varphi \right) \right] \right\}, \qquad (29)$$

where $\lambda = 2g^2/\pi\hbar v_F$ is a dimensionless coupling constant, $\Delta = \Delta_0$, and

$$\tilde{v}_\perp^2 = v_\perp^2 + 4\eta\Delta^2 a_\perp^2/\lambda\hbar^2, \quad \varepsilon_\perp \sim \varepsilon_\Delta (v_F/v_\perp)^{-2} \ll \varepsilon_\Delta.$$

Equation (29) exhibits a general property of theories involving a multifermion vacuum which interacts with external fields, that integration over the fermions always leads to renormalization of the energy of the external field. The components of the permittivity $\hat{\varepsilon}$ automatically appear in the present instance.

Following this remark, it is clear how to generalize the purely Peierls problem to a more realistic case, where there are free charge carriers along with the Peierls subsystem of dielectric electrons. As noted in the Introduction, in a PD, for a variety of reasons, there are always free carriers, as for example due to impurities in the low-temperature phase of TaS_3 (Ref. 14). The mobility of these carriers is greatly diminished by localization effects, but in return they produce the enormous permittivity $\varepsilon_\parallel \sim 10^{6-8} \gg \varepsilon_\Delta$. After integrating over all fermion states, and not just over Peierls states, we can replace ε_Δ by $\varepsilon_\parallel$ in (29). The condition for non-interaction of the localized and Peierls fermion subsystems is $\Delta \gg \hbar/\tau_i$, where τ_j is the characteristic time for an elastic collision with an impurity.

Integrating over χ and making use of the equation

$$\left(\varepsilon_\parallel \frac{\partial^2}{\partial x^2} + \varepsilon_\perp \nabla_\perp^2 \right) \left[\frac{(x-x')^2}{\varepsilon_\parallel} + \frac{|\mathbf{r}_\perp - \mathbf{r}_\perp'|^2}{\varepsilon_\perp} \right]^{-1/2}$$

$$= -4\pi\varepsilon_\parallel^{1/2}\varepsilon_\perp \delta(\mathbf{r} - \mathbf{r}'), \qquad (30)$$

we finally obtain

$$\mathscr{L}_{eff} = \frac{\varepsilon_\parallel E^2}{8\pi} + \frac{n_f}{\pi\hbar v_F}\left\{ \frac{\Delta^2\dot{\varphi}^2}{\lambda\omega_Q^2} - \frac{\hbar^2 v_F^2}{4}(\varphi')^2 - \frac{\hbar^2\tilde{v}_\perp^2}{4}(\nabla_\perp\varphi)^2 \right.$$

$$\left. - eE\hbar v_F\varphi + \frac{2\Delta^2\mu}{4}\cos M\varphi \right\}$$

$$- \frac{e^2}{2\pi} n_f^2 \varepsilon_\perp^{-1}\varepsilon_\parallel^{-1/2} \int d\mathbf{r}'\, \varphi'(x, \mathbf{r}_\perp)\varphi'(x', \mathbf{r}_\perp')$$

$$\left[\frac{(x-x')^2}{\varepsilon_\parallel}+\frac{|\mathbf{r}_\perp-\mathbf{r}_\perp'|^2}{\varepsilon_\perp}\right]^{-1/2}. \tag{31}$$

Taking advantage of the fact that the kernel of the integral depends on the difference $|\mathbf{r}-\mathbf{r}'|$, we rewrite (31) in a more meaningful form:

$$\mathscr{L}_{eff}=N_0\Big\{\dot\varphi^2-c_\parallel^2(\varphi')^2-c_\perp^2(\nabla_\perp\varphi)^2 -\omega_\varphi^2\Big(\varphi+\frac{E}{4\pi E^*}\Big)^2+\frac{2\omega_0^2}{M^2}\cos M\varphi\Big\} +\Gamma\int d\mathbf{r}'(\nabla_\perp\varphi)(\tilde\nabla_\perp\varphi)\left[\frac{(x-x')^2}{\varepsilon_\parallel}+\frac{|\mathbf{r}_\perp-\mathbf{r}_\perp'|^2}{\varepsilon_\perp}\right]^{-1/2}, \tag{32}$$

where

$$N_0=\Delta^2 n_f/\pi\hbar v_F\lambda\omega_Q^2,\ c_{\parallel,\perp}=\hbar v_{F,\perp}\lambda^{1/2}\omega_Q/2\Delta,$$
$$\omega_\varphi^2=\lambda\omega_Q^2\xi_0 2e^2n_f/\pi\varepsilon_\parallel\Delta,\ \omega_0^2=\mu M^2\omega_Q^2,$$
$$\Gamma=e^2n_f^2/2\pi^2\varepsilon_\parallel^{3/2},\ \tilde\nabla_\perp=\partial/\partial\mathbf{r}_\perp',\ E^*=en_f/\pi\varepsilon_\parallel.$$

When $\Delta_\perp\varphi=0$, the Lagrangian (32) is exactly the same as the CDW Lagrangian derived in Ref. 5 using the approximation of the coherent response of a conglomeration of transversely oriented one-dimensional filaments.

ANALYSIS OF THE PHASE EQUATIONS OF MOTION: COHERENCE CRITERION

We can get somewhat of an idea of the role of the Coulomb interaction in phase dynamics by considering the simplest case, that of small phase oscillations. If we assume in the equation of motion for the Lagrangian (32) that $\varphi\sim\exp(ikx+i\mathbf{q}_\perp\mathbf{r}_\perp-i\omega t)$, we obtain

$$\omega^2=\omega_0^2+\omega_\varphi^2+c_\parallel^2k^2+q_\perp^2\Big(c_\perp^2-\frac{\omega_\varphi^2}{q_\perp^2+k^2\varepsilon_\parallel/\varepsilon_\perp}\Big) =\omega_0^2+\omega_\varphi^2\frac{\varepsilon_\parallel}{\varepsilon_\perp}\frac{k^2}{q_\perp^2+k^2\varepsilon_\parallel/\varepsilon_\perp}+c_\parallel^2k^2+c_\perp^2q_\perp^2. \tag{33}$$

It can be seen that the Coulomb term competes with the transverse dispersion, resulting in an effective increase in the transverse stiffness of the system. In fact, with the notation $q_\perp=(\varepsilon_\parallel/\varepsilon_\perp)^{1/2}\tilde q_\perp$, we obtain

$$\omega^2=\omega_0^2+\omega_\varphi^2\frac{k^2}{k^2+\tilde q_\perp^2}+c_\parallel^2k^2+c_\perp^2\frac{\varepsilon_\parallel}{\varepsilon_\perp}\tilde q_\perp^2 \tag{34a}$$

or, with $\tilde k=k(\varepsilon_\parallel/\varepsilon_\perp)^{1/2}$,

$$\omega^2=\omega_0^2+\omega_\varphi^2\frac{\tilde k^2}{q_\perp^2+\tilde k^2}+c_\parallel^2\frac{\varepsilon_\perp}{\varepsilon_\parallel}\tilde k^2+c_\perp^2q_\perp^2. \tag{34b}$$

If $\varepsilon_\perp/\varepsilon_\parallel\ll c_\perp^2/c_\parallel^2$, the zeroth approximation to Eq. (34) is $q_\perp=0$ ($\tilde q_\perp=0$), and we have a small-oscillation dispersion law with plasma activation ω_φ (Ref. 4). From our elementary analysis, we see that for propagation of charge perturbations in a CDW, there is a region $\xi_\perp\sim L_x(\varepsilon_\perp/\varepsilon_\parallel)^{1/2}$ (L_x is the characteristic longitudinal size of a perturbation) within which the phases are correlated across the chains.

The linear treatment does not deal with the basic problem of the structure of the transverse coherence region when soliton-antisoliton pairs are produced by an external field from the CDW condensate. Let us look at the solution of this problem, first recalling where the concept of solitons as current carriers arises.

Consider the ground state of the Lagrangian (32). If we assume that $\varphi=$ const in the ground state, the potential energy density is

$$V(\varphi)=N_0\{\omega_\varphi^2(\varphi+E/4\pi E^*)^2-2\omega_0^2M^{-2}\cos M\varphi\}. \tag{35}$$

With $\omega_\varphi\ll\omega_0/M$, which guarantees the maximum value of $\varepsilon_\parallel$, in fields $E<E_T=4\pi en_f/M\varepsilon_\parallel$, the minimum of $V(\varphi)$ occurs at $\varphi=0$; for $E_T<E<2E_T$, the minimum occurs at $\varphi=-2\pi/M$, for $2E_T<E<3E_T$ it occurs at $\varphi=-4\pi/M$, etc. As the external field varies in an unbounded sample, a new vacuum is locally generated from the old through the formation of nucleation centers satisfying the boundary conditions $\varphi(|\mathbf{r}|<r_0)=-2\pi/M$, $\varphi(|\mathbf{r}|>r_0)=0$ ($E_T<E<2E_T$). When $\varepsilon_\parallel\gg\varepsilon_\perp$, a good approximation for the nucleation center of such a local transition is given by a pair of solutions of the sine-Gordon equation [the one-dimensional Lagrangian (32) for $\omega_\varphi=0$], namely a soliton plus antisoliton moving in opposite directions. At $T=0$, $s\bar s$ pair production proceeds via tunneling along trajectories in imaginary time:

$$\varphi_{s\bar s}=-\frac{4}{M}\Big\{\operatorname{arctg}\exp\Big(-\frac{x+x_0(\tau,\mathbf{r}_\perp)}{d(1+\dot x_0^2/c_\parallel^2)^{1/2}}\Big) +\operatorname{arctg}\exp\Big(\frac{x_0(\tau,\mathbf{r}_\perp)-x}{d(1+\dot x_0^2/c_\parallel^2)^{1/2}}\Big)-\frac{\pi}{2}\Big\}. \tag{36}$$

Here x_0 is the coordinate of the center of the soliton (antisoliton), $d=c_\parallel/\omega_0$ is the soliton width, with $d\ll x_0$. The soliton energy is $U_s=4N_0\omega_0c_\parallel/M^2=8\Delta\mu^{1/2}/\pi M\lambda^{1/2}\gg\omega_0$. The soliton is negatively charged, $\varphi_s'<0$, and the antisoliton is positively charged, $\varphi_{\bar s}'>0$, so the system transition to a new vacuum state is accompanied by the flow of dissipative current.

In the one-dimensional case, where $\varphi(\mathbf{r}_\perp)=$ const, the calculation of the tunneling probability along the instanton trajectory (36) with $x_0=x_0(\tau)$ leads to a nonlinear term in the conductivity (1) (Ref. 5). Then E_T plays the role of a one-dimensional Coulomb field of the soliton barrier. Two questions arise in general: is the ground state homogeneous, and if so, over what region does the soliton profile (36) reduce to the one-dimensional case? Our analysis of the linear mode produces an affirmative answer to the first question, with no instabilities. All of the considerations pertaining to $s\bar s$ nucleation center production remain valid, and we must investigate the equations of motion on the instanton trajectory (36).

Let us look at an example from Ref. 13, which allows us to reduce the Lagrangian (32) to one which depends solely on the field $x_0(\tau,\mathbf{r}_\perp)$. The full CDW Lagrangian is of the form

$$L=\int d\mathbf{r}_\perp dx\,\mathscr{L}_{eff}=\int d\mathbf{r}_\perp n_f l(x_0(\tau,\mathbf{r}_\perp)), \tag{37}$$

$$l=-2U_s\left[1+\frac{\dot{x}_0^2}{c_\parallel^2}\right]^{1/2}+2e^*x_0(E-E_T)$$
$$-U_s\left(\frac{c_\perp}{c_\parallel}\right)^2(\nabla_\perp x_0)^2+\Gamma\int d\mathbf{r}_\perp'(\nabla_\perp x_0)(\tilde{\nabla}_\perp\tilde{x}_0)$$
$$\times\int dx\,dx'\left(\frac{\partial\varphi_{s\bar{s}}}{\partial x_0}\right)\left(\frac{\partial\tilde{\varphi}_{s\bar{s}}}{\partial\tilde{x}_0}\right)\left(\frac{(x-x')^2}{\varepsilon_\parallel}+\frac{|\mathbf{r}_\perp-\mathbf{r}_\perp'|^2}{\varepsilon_\perp}\right)^{-1/2}, \quad (38)$$

where

$$e^*=(2\pi/M)e,\ \tilde{\varphi}_{s\bar{s}}=\varphi_{s\bar{s}}(x',\ x_0(\tau,\ \mathbf{r}_\perp')),\ \tilde{x}_0=x_0(\tau,\ \mathbf{r}_\perp').$$

It is not hard to see, using the representation (31), for example, that since $\delta\varphi_{s\bar{s}}/\partial x_0$ is a sharply peaked function of width $\sim d$, the main contribution to the double integral over x,x' comes from the values of the integrand with $|x-x'|\sim 2x_0$. The contribution from $|x-x'|\sim d$ is a factor $d/x_0\ll 1$ smaller.

If $\Delta_\perp x_0=0$, the Lagrangian (38) is a standard one-dimensional quantum mechanical Lagrangian for a relativistic particle in the field $E-E_T$, and with it, we find the size of the field-induced nucleation center from the condition $\dot{x}_0=0$ on the surface of the bulk sample ($x_0=x^{(0)}$):

$$x^{(0)}=U_s/e^*(E-E_T). \quad (39)$$

We assume that in the general case there is also a region $\sim\xi_\perp$ in which $\Delta_\perp x_0=0$, i.e., for $|\mathbf{r}_\perp'|\ll\xi_\perp$, $x_0=x^{(0)}$, and the Lagrangian is l-dimensional, while for $|\mathbf{r}_\perp'|\gg\xi_\perp$, the one-dimensional Coulomb field disappears. Having estimated $\xi_\perp$ using this condition, we obtain

$$\xi_\perp\ll x^{(0)}(\varepsilon_\perp/\varepsilon_\parallel)^{1/2}\ll x^{(0)}, \quad (40)$$

which is fully consistent with the results of the linear analysis. The previously undefined linear size L_x has acquired the concrete form $L_x\sim x^{(0)}$. Equation (40) still fails to address the question of the structure of $\xi_\perp$, but it confirms that the existence of $\xi_\perp$ does not contradict the assumption (36).

We now find an explicit expression for $\xi_\perp$ by analyzing the stability of the one-dimensional solution for x_0 against transverse (bending) oscillations. We assume that $x_0(\tau,\mathbf{r}_\perp)=x_0(\tau)+\delta x_0(\tau,\mathbf{r}_\perp)$ and write out the equation of motion on the surface of the sample for $x_0=x^{(0)}$, bearing in mind that

$$\delta x_0\sim\exp(i\mathbf{q}_\perp\mathbf{r}_\perp-i\Omega\tau).$$

We obtain

$$\Omega^2=c_\perp^2q_\perp^2\left(1-\frac{q_0}{|q_\perp|}\exp(-2x^{(0)}(\varepsilon_\perp/\varepsilon_\parallel)^{1/2}|q_\perp|)\right),$$
$$q_0=\frac{4\pi}{U_s}\Gamma\varepsilon_\perp^{1/2}(c_\parallel/c_\perp)^2\sim\left(\frac{eE_T}{U_s}\right)\left(\frac{\varepsilon_\perp}{\varepsilon_\parallel}\right)^{1/2}\left(\frac{c_\parallel}{c_\perp}\right)^2. \quad (41)$$

It can be seen that the region $|\mathbf{r}_\perp|\lesssim\xi_\perp$, i.e., $|q_\perp|\gtrsim|q_{\max}|$, exists only when $E>E_T$, and conversely, when $|q_\perp|\to\infty$, $\Omega^2<0$. The size of $\xi_\perp$ is determined by the condition for stability, $\Omega^2=0$, i.e.,

$$1=q_0\xi_\perp\exp(-2x^{(0)}(\varepsilon_\perp/\varepsilon_\parallel)^{1/2}/\xi_\perp). \quad (42)$$

Equation (42) is the required condition for determining the size of the transverse phase-coherence region under conditions of soliton-antisoliton nucleation center production.

According to the inequality (40),

$$\xi_\perp\gtrsim a_\perp(\Delta/\varepsilon_F)^{M/2}\varepsilon_\parallel\bar{v}_\perp/v_F. \quad (43)$$

For the actual parameters of TaS_3, for example, $\xi_\perp\gtrsim 10^2a_\perp$.

Since $\xi_\perp$ depends on the electric field, condition (43) limits the range of variation of E:

$$E_T<E\ll E_T^*=E_T[1+(\varepsilon_\perp/\varepsilon_\parallel)^{1/2}v_F/\tilde{v}_\perp]. \quad (44)$$

As we have seen in the analysis of the linear mode, we have for the ratio $(\varepsilon_\perp/\varepsilon_\parallel)^{1/2}v_F/\tilde{v}_\perp\lesssim 1$, so coherent production of $s\bar{s}$ barriers, and therefore the threshold field-dependence of the conductivity, are only observed in a narrow range about $E_\perp$, which corresponds to the experimental situation.[1]

As noted in the Introduction, the quantity $\xi_\perp$ can be fairly large. If the transverse dimensions of the sample satisfy $L_\perp\lesssim\xi E_\perp$, the current will be coherent everywhere. If the opposite is true, the field-dependence of the tunneling exponent will be governed by respective contributions from coherent and non-coherent portions of the sample. For very thick samples, it is possible for the dependence (1) to be replaced by a different formula lacking a threshold. An exact solution of the boundary problem, which is not yet possible, would provide an answer to this question. Nevertheless, the assumption of random independent $s\bar{s}$ pair production along the chains can obviously be immediately rejected. If we actually take $x_0(\tau,\mathbf{r}_\perp)$ to be a random function with

$$\langle x_0(\tau,\ \mathbf{r}_\perp)\rangle=0, \quad (45)$$

where the angular brackets denote cross-sectional averaging,

$$\langle\ldots\rangle=\int d\mathbf{r}_\perp\ldots, \quad (46)$$

the term in the full Lagrangian (37) associated with the external field simply vanishes, $E\langle x_0\rangle=0$. But this is exactly the term responsible for tunneling. Physically, this means that opposite charges are randomly produced within the system, i.e., there is no mean build-up of charge in the sum.

CONCLUSION

In this paper, we have shown that a quasi-one-dimensional CDW situated in a constant external electric field parallel to the chains is unstable to the production of soliton-antisoliton pairs, which screen the field. Broadly speaking, this instability is of a threshold variety, which is exhibited in samples with small transverse dimensions as a threshold dependence of the nonlinear conductivity on the field.

The structure of $s\bar{s}$ nucleation center production is such that there is always a region of macroscopic dimension $\xi_\perp$ much smaller than the transverse size of a pair, in which the Coulomb field of the soliton and antisoliton is effectively uniform. The size of this region is dictated by competition between dispersion and the Coulomb interaction. In reality, the magnitude of $\xi_\perp$ can be limited either by the size of the sample or structural defects within it. To all appearances, this is in fact the experimental situation, since the field-de-

pendence of $\sigma(E)$ is given by Eq. (1), and in general E_0 also depends on $(E-E_T)$, albeit weakly, since the magnitude of $\xi_\perp$ formally diverges as the field approaches the threshold $E \to E_T$, but it always remains much smaller than the longitudinal size of an $s\bar{s}$ pair. Outside the confines of $\xi_\perp$, the Coulomb field of the $s\bar{s}$ pairs is three-dimensional. The contribution of the coherent region to the tunneling conductivity is determined by the thickness of the sample. In thin samples with $L_\perp \sim \xi_\perp$, we should see a conductivity threshold, while for $L_\perp \gg \xi_\perp$, such a threshold may be lacking. Nevertheless, the threshold field E_T always exists. The properties found by solving the one-dimensional problem[5] are preserved in the quasi-one-dimensional case, and are consistent with what is observed experimentally.

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