Quasi–one-dimensional charge density wave in electromagnetic field arbitrary oriented to conducting chains: Generalized Fröhlich relations

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Abstract. – We derive equations for the collective CDW-current transverse conducting chains in a quasi–one-dimensional CDW conductor. Generalized Fröhlich relations between the transverse currents and phase gradients are due to the polarization corrections to the 1 + 1 chiral anomaly Lagrangian. The CDW Hall constant $R_{\text{CDW}}$ is calculated, $R_{\text{CDW}} \sim T_C^2/I_{\text{CDW}}$, where $T_C$ is the critical temperature of the Peierls transition, and $I_{\text{CDW}}$ is the nonlinear CDW current in the direction parallel to the conducting chains.

The Quasi-One-Dimensional (Q1D) Charge Density Wave (CDW) conductors such as NbSe\textsubscript{3}, TaS\textsubscript{3}, K\textsubscript{0.3}MoO\textsubscript{3} etc. (see, for instance, ref. [1]) are characterized by a strongly anisotropic quasiparticle spectrum. As a result, their unusual transport properties are mostly pronounced in the direction parallel to the conducting chains. The theoretical studies of the CDW electrodynamics were mainly focused on the one-dimensional aspect. The response of a 1D CDW is described by the well-known Fröhlich relations [1]

$$j_x = -\frac{e}{\pi x} \frac{\partial \varphi}{\partial t} n_f , \quad \rho = \frac{e}{\pi x} \frac{\partial \varphi}{\partial x} n_f ,$$

(1)

where $j_x$ is the collective current density along the direction of the chains, $\rho$ is the charge density fluctuation, $n_f$ is the density of chains and $\varphi$ is the CDW variable, the phase of the

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Peierls-Fröhlich order parameter $\Delta \exp[i\varphi]$. The amplitude $\Delta$ is equal to the gap width in the single-particle spectrum.

Experimental investigations of the transverse CDW transport, and in particular of the Hall effect [2,3], have demonstrated that the 3D effects are also strongly affected by the nonlinear CDW transport current $I_{\text{CDW}}$ directed along the chains. It was found in ref. [3] that the Hall constant $R_{\text{CDW}}$ is proportional to $I_{\text{CDW}}^{-1}$ and sharply decreases in electric fields above the threshold $E_T$. This fact is not yet explained within the microscopic theory. To describe properly the 3D electrodynamics of CDW, we need the generalized Fröhlich equations for all three components of the collective current $I_{\text{CDW}}$. This problem is solved in the present paper, and the dependence of $R_{\text{CDW}}$ on $I_{\text{CDW}}$ is obtained.

The description of a Q1D CDW is based on the electron-lattice Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2M} \sum_{\vec{n}_\nu} \frac{\partial^2}{\partial u_{\vec{n}_\nu}^2} + \sum_{\vec{n}_\nu} K_{\nu} \left(u_{\vec{n}_\nu} - u_{\vec{n}_{\nu+1}}\right)^2 + \sum_{\vec{n}_\nu} \left(t_\nu + t_{1\nu} \left(u_{\vec{n}_\nu} - u_{\vec{n}_{\nu+1}}\right)\right) \left(a_{\vec{n}_\nu,s} a_{\vec{n}_{\nu+1},s} + \text{h.c.}\right),$$

where $u_{\vec{n}}$ is the lattice displacement, $\vec{n}$ numerates lattice sites, $\nu = x, y, z$, $M$ is the ion mass, $K_{\nu}$ are the lattice elasticity constants, $t_\nu$ is the electron hopping integral, $t_{1\nu}$ is the electron-lattice coupling, $a_{\vec{n}s}$ and $a_{\vec{n}s}$ are the creation and annihilation operators of an electron with spin $s$ at the site $\vec{n}$.

The Q1D approximation is formulated as follows:

$$u_{n_x} = u_0 \cos(2kFn_x b_x + \varphi),$$
$$a_{\vec{n}s} = \Psi_{R,s} \exp[ikFn_x b_x] + \Psi_{L,s} \exp[-ikFn_x b_x],$$
$$u_{\vec{n},y,z} - u_{\vec{n}+\vec{t}_{y,z}} \simeq \frac{\partial u_{\vec{n}}}{\partial y(z)} b_{y,z},$$
$$t_{1y,z} = 0. \quad (3)$$

For our purposes, it is convenient to formulate the theory in the Lagrange formalism.

After the standard redesignations (see, e.g., [4]):

$$b_x t_0 = \hbar V_F, \quad 2t_1 u_0 / b_x = \Delta, \quad K_x b_x \sin^2(b_x k_F) / 16 t_{1x}^2 = \frac{1}{g^2},$$

the Peierls-Fröhlich Lagrangian takes the form ($\hbar = c = 1$)

$$\mathcal{L} = \varphi \left(\frac{1}{\alpha^2 V_F} \partial_x^2 - \frac{U_x^2}{V_F} \partial_y^2 - \frac{U_y^2}{V_F} \partial_z^2\right) \varphi - \frac{\Delta^2}{2g^2} + \psi \{i\sigma_2 (\partial_t + ie\Phi) + it_x \text{ch}(b_y (\partial_y - ieA_y))\} + \psi \bar{\sigma}_1 V_F (\partial_x - ieA_x) - \Delta \exp[-i\sigma_3 \varphi] \psi = \mathcal{L}^{\text{ph}} + \bar{\psi} L \psi, \quad (4)$$

where the electromagnetic field is introduced in a gauge-invariant form. Here $\alpha^2 \equiv \frac{\Delta}{V_F M}$, $\alpha$ is the adiabatic parameter of the Peierls-Fröhlich theory [4], $U_{y,z}$ are the transverse phonon velocities, $\Phi$ and $A_\nu$ are the scalar and vector potentials, $\psi^\dagger = (\psi_{R}^\dagger, \psi_{L}^\dagger)$, $\bar{\psi} = \psi^\dagger \sigma_2$ and $\sigma_\nu$ are the Pauli matrices. Note that the approximation (3) which leads to eq. (4) is well defined only when $t_{y,z} \ll \Delta$.

The CDW currents are

$$j_\nu = c \frac{\delta F}{\delta A_\nu}, \quad \rho = -\frac{\delta F}{\delta \Phi}, \quad (5)$$
where $F$ is the free energy:

$$F = -T \ln \int D\Delta D\varphi D\bar{\psi}D\psi \exp \left[ \int_0^\infty d\tau \int d\vec{r} \mathcal{L}_E \right] =$$

$$-T \ln \int D\Delta D\varphi D\exp \left[ \int_0^\infty d\tau \int d\vec{r} \mathcal{L}_E^{\mathrm{ph}} + \mathrm{Tr} \ln L_E \right]$$

(6)

Here $\mathcal{L}_E$ is the Euclidean Lagrangian, $\tau = -it$, $T$ is the temperature and $\mathrm{Tr}\hat{O} = 2\mathrm{Tr} \int d\vec{r} \langle \hat{O} | \hat{O} \rangle$, where $\mathrm{Tr}$ denotes trace over the matrix indices, and the multiplier 2 results from the summation over the electronic spins.

To calculate $\mathrm{Tr} \ln L_E$, we perform the chiral rotation

$$\psi \rightarrow \exp \left[ -\frac{i\sigma_3}{2} \varphi \right] \bar{\psi}, \quad \bar{\psi} \rightarrow \bar{\psi} \exp \left[ i\frac{\sigma_3}{2} \varphi \right].$$

(8)

Then

$$\exp[\mathrm{Tr} \ln L_E] = J\{\varphi\} \exp[\mathrm{Tr} \ln \hat{L}_E],$$

(9)

where $J\{\varphi\}$ is the functional Jacobian and the Lagrangian $\hat{L}_E$ is

$$\hat{L}_E = \left\{-\sigma_2 \left[ \partial_\tau + \frac{V_F}{2} \partial_x \varphi + e\Phi + t_y \text{ch}(b_y(\partial_y - ieA_y)) + t_z \text{ch}(b_z(\partial_z - ieA_z)) \right] - \sigma_1 V_F \left[ \partial_x - \frac{1}{2V_F} \partial_x \varphi - ieA_x \right. \right.$$

$$\left. - \frac{t_y b_y}{2V_F} \partial_x \varphi \text{sh}(b_y(\partial_y - ieA_y)) - \frac{t_z b_z}{2V_F} \partial_z \varphi \text{sh}(b_z(\partial_z - ieA_z)) \right] - \Delta \right\},$$

(10)

at $b_y\partial_y \varphi, b_z\partial_z \varphi \ll 1$.

We calculate the Jacobian following the Fujikawa scheme [5]. According to this

$$J^{-1}\{\varphi\} = \exp \left[ -\frac{1}{2} \int d\vec{r} d\tau \mathrm{Tr} \chi^* \sigma_3 \chi \right],$$

(11)

where $\chi$ stands for the complete set of the asymptotic eigenfunctions of the Lagrangian $\hat{L}_E$ taken in the ultraviolet limit, i.e. at the energies far exceeding $e\phi, eA_xV_F, t_y, z$, and $\Delta$:

$$\chi = \exp \left[ i(k_x x + \omega \tau + k_y y + k_z z) \right].$$

(12)

We have

$$\mathrm{Tr}(\chi^* \sigma_3 \chi) = 2 \lim_{N \rightarrow \infty} \frac{1}{(2\pi)^4} \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dw \int_{-\pi/b_y}^{\pi/b_y} dk_y \int_{-\pi/b_z}^{\pi/b_z} dk_z \chi^* \exp \left[ \frac{\hat{L}_E \sigma_3 \hat{L}_E \sigma_3}{N^2} \right] \chi =$$

$$= \frac{2}{b_y b_z} \left\{ -\frac{1}{2V_F} \partial_x^2 \varphi - \frac{V_F}{2\pi} \partial_x \varphi - \frac{e}{\pi} E_x + \frac{V_y^2}{2V_F} \partial_y^2 \varphi + \frac{V_z^2}{2V_F} \partial_z^2 \varphi \right\} -$$

$$- \frac{e b_y t_y}{2V_F} \left( \text{ch}(b_y(\partial_y - ieA_y)) \right) \left( E_y - \frac{1}{2e} \partial_y^2 \varphi \right) \partial_y \varphi - (y \rightarrow z) -$$

$$- i e b_y t_y \left( \text{sh}(b_y(\partial_y - ieA_y)) \right) \left( H_z + \frac{1}{2V_F e} \partial_z^2 \varphi \right) - (y \rightarrow z).$$

(13)
\[ \langle \hat{f} \rangle = \int dk_x dk_y dk_z d\omega \chi^* \hat{f} \chi, \]

and \( E_\nu, H_\nu \) are electric and magnetic fields. It is readily seen that

\[ \langle ch(b_\nu(\partial_\nu - ieA_\nu)) \rangle = \langle sh(b_\nu(\partial_\nu - ieA_\nu)) \rangle = 0 \]

and the Jacobian takes the form

\[ J\{\varphi\} = \exp \left[ - \int d\vec{r} \, d\tau l\{\varphi\} \right], \]

where

\[ l\{\varphi\} = \frac{1}{b_y b_z} \left\{ \frac{1}{4V_F^2} (\partial_x \varphi)^2 + \frac{V_F}{4\pi} (\partial_y \varphi)^2 - \frac{V_y^2}{4\pi V_F} (\partial_\nu \varphi)^2 - \frac{\mu_{zz}}{\pi} E_x^2 - \frac{\mu_{yy}}{\pi} E_y^2 \right\}, \]

In a 1D CDW \((V_y = V_z = 0)\), the Lagrangian (17) coincides with the one for the chiral anomaly in 1+1 massless quantum field theory (see, e.g., [6]). The connection between the 1D CDW Lagrangian and the chiral anomaly phenomenon was demonstrated in refs. [7, 8]. The Fröhlich relations (1) evidently follow from the Lagrangian (17).

So, in a Q1D CDW, the chiral anomaly mechanism gives the wrong sign only in the transverse dispersion in eq. (17). The normal CDW dispersion is restored due to the phonon terms in the Lagrangian (4) [9]. A modification of Fröhlich relations arises due to the polarization terms in the free energy hidden in \( \text{Tr} \ln \tilde{L}_E \) (eq. (9)).

In ref. [10] the chiral anomaly was studied in a formally similar system: the Q1D spin density wave. It was claimed in [10] that, under the conditions of a quantum Hall effect, the chiral anomaly produces additional terms linear in \( t_y \) in eqs. (1). In this paper, we study the opposite limit of classically “weak” magnetic fields (eq. (15)) when the terms linear in \( t_{y,z} \) turn to zero.

Consider \( \text{Tr} \ln \tilde{L}_E \) at \(|E|, |H| \ll \Delta^2 / eV_F \) and \( \partial \varphi \ll \Delta / V_F, \partial \tau \varphi \ll \Delta \). The straightforward perturbation expansion (see, e.g., [4]) gives

\[ \text{Tr} \ln \tilde{L}_E = \frac{1}{2} \text{Tr} \ln \tilde{L}_E \sigma_3 \tilde{L}_E \sigma_3 \cong \]

\[ \cong \frac{1}{2} \ln \tilde{K}_0 - \frac{1}{2} \int d\vec{r} d\tau \left\{ \kappa_{xx} \tilde{E}_x^2 + \kappa_{yy} \tilde{E}_y^2 + \kappa_{zz} \tilde{E}_z^2 + \mu_{zz} \tilde{H}_z^2 + \mu_{yy} \tilde{H}_y^2 \right\}. \]

Here

\[ \tilde{K}_0 = -\partial_x^2 - V_F^2 \partial_y^2 + \Delta^2, \]

and

\[ \kappa_{xx} = \frac{1}{8\pi^2 \Delta^2}, \quad \kappa_{yy,zz} = \kappa_{xx} \left( \frac{t_{y,z}}{\epsilon_F} \right)^2 \ll \kappa_{xx}, \]

\[ \mu_{yy} \sim \left( \frac{V_F}{c} \right)^2 \kappa_{zz}, \quad \mu_{zz} \sim \left( \frac{V_F}{c} \right)^2 \kappa_{yy} \]

are the diagonal components of the tensor of the dielectric and magnetic susceptibilities, \( \omega_p = (8e^2 V_F / \Delta^2 b_y b_z)^{1/2} \) is the plasma frequency, \( \epsilon_F = V_F / b_x \) is the Fermi energy, and
\[ \tilde{E}_x = E_x - \frac{1}{2V_F} \partial_x^2 \varphi - \frac{V_F}{2e} \partial_x^2 \varphi, \]
\[ \tilde{E}_y = E_y - \frac{V_F}{2e} \partial_{x,y} \varphi, \]
\[ \tilde{E}_z = E_z - \frac{V_F}{2e} \partial_{z}^2 \varphi, \]
\[ \tilde{H}_y = H_y + \frac{i}{2V_F} \partial_{yz}^2 \varphi, \]
\[ \tilde{H}_z = H_z + \frac{i}{2V_F} \partial_{yz}^2 \varphi. \] (21)

Finally, we substitute eqs. (18) and (16) into eq. (6) and calculate the variation of the free-energy functional with respect to the vector and scalar potentials to obtain currents in accordance with eq. (5). We get in real time
\[ j_x = -\frac{e}{\pi b_y b_z} \partial_y \varphi - \frac{\kappa_{xy} V_F}{2e} \partial_x \left( \partial_x^2 \varphi - \frac{1}{V_F^2} \partial_x^2 \varphi - \frac{V_y^2}{V_F^2} \partial_y^2 \varphi - \frac{V_z^2}{V_F^2} \partial_z^2 \varphi \right) + \]  
\[ + \frac{\kappa_{yy} V_F}{2e} \partial_{yy}^3 \varphi + \frac{\kappa_{zz} V_F}{2e} \partial_{zz}^3 \varphi, \]
\[ \rho = \frac{e}{\pi b_y b_z} \partial_x \varphi - \frac{\kappa_{xx} V_F}{2e} \partial_x \left( \partial_x^2 \varphi - \frac{1}{V_F^2} \partial_x^2 \varphi - \frac{V_y^2}{V_F^2} \partial_y^2 \varphi - \frac{V_z^2}{V_F^2} \partial_z^2 \varphi \right) + \]  
\[ + \frac{\kappa_{xy} V_F}{2e} \partial_{xy}^3 \varphi + \frac{\kappa_{zz} V_F}{2e} \partial_{zz}^3 \varphi, \] (22)
\[ j_y = -\frac{\kappa_{yy} V_F}{e} \partial_{yy}^3 \varphi, \]
\[ j_z = -\frac{\kappa_{zz} V_F}{e} \partial_{zz}^3 \varphi. \] (23)

It is evident that eqs. (23)-(25) automatically satisfy the condition \( \partial_t \rho + \text{div} \vec{j} = 0 \).

It is easy to check from the equation of motion
\[ \frac{\delta}{\delta \varphi} \left\{ \int d\vec{r}dt[L^\text{ph} + l\{\varphi\}] + \text{Tr ln} \hat{L} \right\} = 0, \] (26)

that the polarization correction to eq. (26), as well as to \( j_x \) (23) and \( \rho \) (23), can be safely neglected in electric fields \( |\vec{E}| \ll e^2/4\pi\kappa_{xx}\Delta^2 \). As actually \( \kappa_{xx} \simeq 1 \), this inequality always holds in experiment.

Hence, the incommensurate Q1D CDW is described by the equation of motion
\[ \frac{1}{\alpha^2} \partial_t^2 \varphi - \frac{V_F^2}{2} \partial_x^2 \varphi - \frac{U_y^2}{2} \partial_y^2 \varphi - \frac{U_z^2}{2} \partial_z^2 \varphi = \frac{e}{\pi} E_x, \] (27)

by the Maxwell equations and by the generalized Fröhlich relations
\[ j_x = -\frac{e}{\pi b_y b_z} \partial_y \varphi + \frac{\kappa_{yy} V_F}{2e} \partial_{yy}^3 \varphi + \frac{\kappa_{zz} V_F}{2e} \partial_{zz}^3 \varphi, \]
\[ \rho = \frac{e}{\pi b_y b_z} \partial_x \varphi - \frac{\kappa_{xx} V_F}{2e} \partial_x \left( \partial_x^2 \varphi - \frac{1}{V_F^2} \partial_x^2 \varphi - \frac{V_y^2}{V_F^2} \partial_y^2 \varphi - \frac{V_z^2}{V_F^2} \partial_z^2 \varphi \right) + \]  
\[ + \frac{\kappa_{xy} V_F}{2e} \partial_{xy}^3 \varphi + \frac{\kappa_{zz} V_F}{2e} \partial_{zz}^3 \varphi, \]
\[ j_y = -\frac{\kappa_{yy} V_F}{e} \partial_{yy}^3 \varphi, \]
\[ j_z = -\frac{\kappa_{zz} V_F}{e} \partial_{zz}^3 \varphi. \] (28)
As an application of our formulas (27), (28), we calculate the Hall constant of the CDW condensate at zero temperature.

Consider the Hall geometry: \( H = H_z \), the transport CDW current \( I_x \) flows parallel to the chains in a film with sizes \( L_y, L_z \). As normally \( t_z \ll t_y \), we neglect the \( z \)-dependence in eqs. (27), (28). Performing the perturbation expansion over \( \kappa_{yy} \) in Maxwell equations, we get

\[
E_y = -2\pi \kappa_{yy} \frac{V_F}{e} \frac{\partial^2 \phi}{\partial y^2}, \quad H_z = H_0,
\]

where \( H_0 \) is the external magnetic field which is assumed to be larger than the magnetic field of the transport current.

In sliding CDW \( \phi = \phi(x - V_D t, y, z) \), where \( V_D(E_x) \) is the nonlinear drift velocity. We get

\[
E_y = \frac{2\pi \kappa_{yy} V_F}{e^2} \frac{b_y b_z}{V_D} \frac{\partial j_x}{\partial y}.
\]

The Hall constant is

\[
R_{CDW} = \int_0^{L_y} \frac{dy E_y}{c H_z I_x} = \frac{2\pi^2 \kappa_{yy}}{cc^2 H_0} \frac{V_F}{V_D(E_x)} \frac{b_y b_z}{L_z}.
\]

Hence

\[
R_{CDW} I_x(E_x) = \text{const} \sim t_y^2 \sim T_C^2,
\]

where \( T_C \) is the temperature of the Peierls transition. The r.h.s. in eq. (32) is independent of \( E_x \) which is in a good accordance with the experimental data [3].

**Conclusion.** – We have derived for the first time the generalized Fröhlich relations which relate the transverse currents and fields to the phase gradients in a Q1D CDW conductor. The explanation of the relation between the CDW Hall constant and the nonlinear transport current is found.

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