Convective Term and Transversely Driven Charge-Density Waves

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Abstract

We derive the convective terms in the damping which determine the structure of the moving charge-density wave (CDW), and study the effect of a current flowing transverse to conducting chains on the CDW dynamics along the chains. In contrast to a recent prediction we find that the effect is orders of magnitude smaller, and that contributions from transverse currents of electron- and hole-like quasiparticles to the force exerted on the CDW along the chains act in the opposite directions. We discuss recent experimental verification of the effect and demonstrate experimentally that geometry effects might mimic the transverse current effect.

PACS numbers: 71.45.Lr, 72.15.-v, 72.20.Pa
Nonequilibrium steady states of driven periodic systems with quenched disorder have attracted significant interest. Examples include quasi-1D charge-density waves (CDW),\(^1\) vortex lattices in superconductors,\(^2\) two-dimensional Wigner crystals.\(^3\) All these systems are characterized by pinning, so that macroscopic motion is only set up when the applied force is larger than a threshold value.

In the particular case of quasi-1D CDW where the CDW motion is only along the chains, many interesting effects were predicted,\(^4\)–\(^6\) such as a dynamical phase transition between a disordered and an ordered state and instability due to the proliferation of phase slips. While a dynamic transition was observed in the recent experiment on high-quality NbSe\(_3\) crystals,\(^7\) between temporally ordered CDW creep to high-velocity sliding, many of the predicted effects have not yet been detected. The predictions were based on the equation of motion including a phenomenological convective term in the damping, \(\gamma[\partial_t \varphi + (v \nabla) \varphi]\), where \(v\) stands for the velocity of the moving lattice (in our case for the CDW velocity).

Recently Radzihovsky and Toner\(^8\) predicted a dramatic effect of transverse current on CDW motion along the conducting chains. This effect results in a "current-effect transistor" in which the CDW channel is turned on by a transverse quasiparticle current. The effect, again, stemmed from a convective term phenomenologically inserted in the equation of CDW motion, the velocity \(v\) being assumed to be of the order of the normal electron velocity. An experimental verification of this effect was reported recently by Markovic \textit{et al}.\(^9\)

The convective term introduced in ref.\(^8\) has a different origin from that of refs.\(^4\)–\(^6\). In the former case such a term reflects the action of the transverse current on the CDW, in the latter case it appeared because Galilean invariance was implicitly assumed for damping, and the time derivative \(\partial_t\) was replaced by the convective derivative \(\partial_t + v \partial_x\). This would be valid if damping in the laboratory frame were the same as in the frame moving with the CDW. CDW damping is induced by scattering of quasiparticles, thus the scattering would be the same in both frames if the scatterers (impurities and phonons) were moving with the CDW. Since it is not so, calculation of the damping coefficient from the microscopic theory is needed. The explicit calculation\(^10\) yields neither Galilean invariance nor the convective term. Nevertheless, terms with such a symmetry are allowed, and terms resembling the convective one appear for a completely different physical reason, namely, due to local perturbations of the quasiparticle density. We discuss this problem shortly below.

The main purpose of our paper is to elucidate the physical origin and to derive the convective term by means of the microscopic transport theory\(^10\). We find that this term is orders of magnitude smaller than it was proposed in ref.\(^8\); furthermore, it is proportional to the \textit{difference} of transverse electron and hole currents rather than to the total transverse current. Thus the net force acting on the CDW is determined by the difference of quasiparticle contributions from energies above and below the Fermi surface, like in the Hall effect or thermopower. In principle, predictions of ref.\(^8\) survive, but the effects become much smaller. As for the experimental verification of this effect,\(^9\) we show that a similar behavior may be caused by quite large longitudinal current induced by the transversely applied voltage due to the large anisotropy of CDW compounds.

Though we study here the CDW only, we expect that our conclusions are qualitatively valid for other types of moving periodic structures. In these systems the damping is related to quasiparticle scattering as well, and the Galilean invariance does not hold, so the longitudinal convective term must be proved by a microscopic theory. As for the transverse effect in
related systems, we expect that it must also be related to the difference between the electron and hole current rather than to the total current, as well.

To derive the equation of motion for the CDW phase we start from the equation for the nonequilibrium quasiclassical Green’s functions in Keldysh representation which we use in discrete form with respect to chain indices. The Green’s functions

\[
\hat{g}(t_1, t_2) = \begin{pmatrix} \hat{g}^R(t_1, t_2) & \hat{g}^K(t_1, t_2) \\ 0 & \hat{g}^A(t_1, t_2) \end{pmatrix}
\]

are formed by the retarded and advanced Green’s functions and by \( \hat{g}^K \) which is responsible for the electron distribution. Each of \( \hat{g}^I \) is a matrix with respect to the index identifying the sheets of the Fermi surface of the quasi-one-dimensional conductor at \(+p_F\) and \(-p_F\), and to the chain number. They satisfy the equation (in units with \( c = 1, h = 1 \))

\[
iv_F \partial_x \hat{g}_{nm} + \sum_i t_{\perp i} [A_{nn+i}(t_1)\hat{g}_{n+i,m} - \hat{g}_{n,m+i}A_{n+i,m}(t_2)] + h_n(t_1)\hat{g}_{nm} - \hat{g}_{nm}h_n(t_2) + \Sigma_n\hat{g}_{nm} - \hat{g}_{nm}\Sigma_m = 0,
\]

where matrix product and the convolution with respect to time in the last terms presenting the elastic collision integral are assumed, \( h_n = i\sigma_z\partial_t + i\sigma_y\Delta_n - \Phi_n\sigma_z, \Phi_n = \phi_n - (v_F/2)\partial_x\phi_n, \phi_n \) is the electric potential, \( \Delta_n \) and \( \varphi_n \) are the CDW amplitude and phase, \( \Sigma_n = \frac{1}{4}v_F\sigma_z\hat{g}_{nn}\sigma_z - \frac{1}{4}\nu_b[\sigma_x\hat{g}_{nn}\sigma_x + \sigma_y\hat{g}_{nn}\sigma_y], \nu_f \) and \( \nu_b \) are the forward- and back-scattering rates. The term with \( t_{\perp} \) describes the interchain coupling. \( A_{nm} = \sigma_z \cos \frac{\varphi_{n,m}}{2} + i \sin \frac{\varphi_{n,m}}{2}, \varphi_{n,m} = \varphi_n - \varphi_m. \)

Equation for the phase can be found from the self-consistency conditions for the order parameter.

\[
\text{Tr}\sigma_x\hat{g}^K_{nn}(t, t) = \frac{i m^*}{m} \frac{1}{\Delta} \partial^2\varphi_n.
\]

We solve equation (1) perturbatively with respect to \( t_{\perp} \). The function \( \hat{g}^K_{nn} \) we present as a sum of regular and anomalous parts, the latter is related to nonequilibrium perturbations of the quasiparticle distribution function. \( \hat{g}^K_{nn} = \hat{g}^R_{nn}t_{m} - \hat{g}^A_{nn}t_{n} + \hat{g}^{(a)}_{nn}, t_{n} = 1 - 2n_F(\epsilon - \mu_n), n_F \) is the Fermi distribution function, \( \mu_n \) is the shift of the chemical potential in chain \( n \), and \( \epsilon \) is the energy related to \( t_1 - t_2 \) by Fourier transformation.

In the zeroth approximation we neglect \( t_{\perp} \) and find \( \hat{g}^{R(A)}_{nn} = g_n\sigma_z + f_ni\sigma_y, g^{(a)}_{nn} = 0 \) with \( g_n = \epsilon_n/\xi_n, f_n = \Delta_n/\xi_n, \epsilon_n = \epsilon - \Phi_n + iv_f g^{R(A)}_n/2, \nu_f = \nu_f + \nu_b, \Delta_n = \Delta_n - i\nu_f g^{R(A)}_n/2, \xi_n^{R(A)} = \pm \sqrt{\epsilon_n^2 - \Delta_n^2}. \)

In the first approximation we calculate Green’s functions off-diagonal with respect to layer indices.

\[
\hat{g}^{(a)}_{nn+i} = \sum_i t_{\perp i}(t_n - t_{n+i}) (A_{nn+i} - \hat{g}^R_{nn+i}A_{n+i,n}g^{A}_{n+i,n+i}),
\]

the result for retarded (advanced) function can be obtained from (3) by substituting \( (t_n - t_{n+i}) \) by 1, and all indices \( A \) for \( R \) (\( R \) for \( A \)).

Using (3) we can calculate the transverse current.

\[
\hat{j}_{n,n+1}(x) = \frac{iv_F^2}{64\pi} \sum_i t_{\perp i} \text{Tr}(A_{nn+i}\hat{g}^K_{n+i,n} - \hat{g}^K_{nn+i}A_{n+i,n})d\epsilon,
\]
where $\kappa$ is the inverse Thomas-Fermi screening radius. In the linear approximation with respect to the driving field, $E_\perp = (V_n - V_{n+1})/d$, related to the difference of electrochemical potentials, $V_n = \Phi_n - \mu_n$, we get for the simplest case of identical chains and temperatures $T \ll \Delta$

$$j_{n,n+1}(x) = \sigma_\perp E_\perp,$$

$$\sigma_\perp = \sigma_{\perp N} \frac{\nu_+}{2\nu} \left( \cos^2 \frac{\varphi_{n,n+1}}{2} + \frac{2T}{\Delta} \right) e^{-\Delta/T} \sinh \frac{\mu}{T},$$

where $\nu_+ = \nu_f + \nu_b$, $\nu = \nu_f + \nu_b$, $\sigma_{\perp N}$ is the normal-state conductivity. Under typical experimental conditions the phase in the transverse directions varies over large distances and one can substitute $\varphi_{n,n+1}$ for zero.

If some chains are not in the Peierls state, like in NbSe$_3$, an additional contribution to the conductivity appears, which is related to the hopping between the chains in the metallic state and exhibits no thermal activation.

The second order corrections in $t_\perp$ to $\hat{g}_{mn}$ we calculate by inserting the first order correction (3) into equation (1) for $n = m$. After some algebra we get the component of Green's function $g_x = \mathrm{Tr} \hat{g}^K_{mn}$ needed to calculate the equation for the phase by means of eq.(2). In addition to standard terms describing the elastic deformation, action of the electric field and damping of the CDW which can be found in refs. 10,11, this function contains the term which is related to perturbations of the quasiparticle distribution function by the transverse quasiparticle flow. This additional term reads

$$g_{x\perp}^{(a)} = \sum_i i t_{\perp i}^2 (V_{n+i} - V_n) \sin \varphi_{n,n+i} G(\varepsilon),$$

$$G = \frac{d\mu_n}{d\varepsilon} \mathrm{Re} \frac{f_n^R [\xi_n^R + (\xi_n^A + \xi_{n+i}^R)(g_n^R g_n^A - f_n^R f_n^A)]}{(\xi_n^R + \xi_n^A)(\xi_n^R + \xi_{n+i}^R)(\xi_n^A + \xi_{n+i}^R)}.$$  

Integration of expression (4) over energy gives the force induced by the transverse currents. Note that in $G(\varepsilon)$ the derivative of the Fermi distribution functions is multiplied by an odd function of energy. This means that the contributions of electrons ($\varepsilon > 0$) and holes ($\varepsilon < 0$) have different signs. If the chemical potential is not shifted from the midgap position, i.e. $\mu = 0$, then the electron and hole contributions compensate each other, and the convective term disappears. If $\mu \neq 0$ then this compensation is not complete. For brevity we assume the condition $T \ll \Delta$ which typically holds in CDW conductors practically at all temperatures below the fluctuation region near the Peierls transition. Then the equation for the phase acquires the form

$$\frac{m*}{m} \frac{\partial^2 \varphi_n}{\partial t^2} + \gamma \frac{\partial \varphi_n}{\partial t} - v_F^2 \frac{\partial^2 \varphi_n}{\partial x^2} + 2 \sum_i t_{\perp i}^2 [1 + A(V_n - V_{n+i})] \sin \varphi_{n,n+i} = F_{\text{pin}} + 2v_F E_n,$$

where $A = (\Delta_n/2) \int G(\varepsilon) d\varepsilon$, and $F_{\text{pin}}$ is a pinning force. In the continuous approximation equation the last term in the left-hand side of (6) reads $v_F^2 [\nabla^2 \varphi + 2A(E_\perp \nabla_\perp) \varphi]$, where $v_F^2 = (t_\perp d)^2/2$, $d$ is the interchain distance. The term with $A$ is the convective term describing the transverse effect. Coefficients $\gamma$ and $A$ in the equation depend on details of the energy
structure of the compound, e. g. on energy dependence of the density of states etc. Noting that the main contribution to the integrals stems from the energies close to the gap edge, we simplify (I) in two limits, $p = (\Delta \nu^2)^{1/3}/T \ll 1$ and $p \gg 1$. With the accuracy of a factor of the order of unity we get

$$
\gamma \sim 2\nu_b \frac{\Delta}{T} \left\{ \ln \frac{1}{p} \right\} e^{-\Delta/T} \cosh \frac{\mu}{T},
$$

$$
A \sim \frac{1}{\nu} \left\{ p \right\} e^{-\Delta/T} \sinh \frac{\mu}{T} \text{ at } \left\{ \frac{p}{1} \gg 1 \right\}
$$

(7)

Both the damping factor $\gamma$ and the convective term exhibit a thermally activated behavior because they are related to excitations via the Peierls gap. If some chains are not in the Peierls state, non-thermally activated contributions appear in the next order approximations in $t_\perp/\Delta$. This happens due to proximity effect which induces non-zero density-of-states inside the gap at the chains in the Peierls state and to CDW correlations at the chains in the metallic state. Such contributions are of the order of $\nu_b \mu^2/\Delta^2$ to factor $\gamma$, and of the order of $t_\perp^2 \mu/\Delta^4$ to coefficient $A$. Though these contributions are small they may become dominant since contributions (I) are thermally activated and may be very small.

Eq.(7) shows that the local value of the damping coefficient depends on a local variation of the chemical potential, the latter being related to a local perturbation of the quasiparticle density $\delta n/n$

$$
\gamma = \gamma_0 (1 + a \delta n/n),
$$

where $a$ is a factor of order 1. The last term can be presented in the form of a convective term with the velocity parallel to the CDW motion. We present a "quick and dirty" qualitative derivation of such a term. Let us consider the regime of linear screening when the shift of the chemical potential $\delta \mu$ from the equilibrium position is small. Then we estimate $\delta n/n \sim \delta \mu/T$ in a semiconducting CDW state, and $\delta n/n \sim \delta \mu/E_F$ in the metallic CDW state, where $E_F$ is the Fermi energy. $\delta \mu$ can be found from the quasineutrality condition.

The local perturbation of the charge density consists of the CDW and the quasiparticle contribution, $\rho \propto [N_c v_F \partial_x \varphi + \mu n_c (1 - N_c) \delta \mu]$, where $N_c$ is the fraction of electrons condensed in the CDW. Then, expressing $\delta \mu$ from the condition $\rho = 0$ and inserting it to (8), we find the renormalisation of the damping term. Using the standard expression for the CDW velocity $v = \partial_t \varphi/2k_F$ we present the damping term for the metallic CDW in the form resembling the convective derivative

$$
\gamma = \gamma_0 \left( \partial_t \varphi + b \frac{N_c}{1 - N_c} v \partial_x \varphi \right).
$$

(9)

The "convective" term here is proportional to the temperature dependent ratio between contribution of the condensed electrons and quasiparticles, which is small in NbSe$_3$ or $m$-TaS$_3$ for the upper CDW region. In the case of semiconducting CDW the additional factor $E_F/T$ in the "convective" term appears, and since typically $(1 - N_c) \ll 1$ the renormalisation of the damping coefficient is large. Note, however, that in refs. the convective term contains an averaged CDW velocity, while in Eq.(2) $v$ is the time and position dependent local CDW velocity which can be treated as a constant parameter only in the limit of large CDW velocity.
Thus electric fields induced by local perturbations of the quasiparticle density renormalize the damping similarly to renormalization of the quasiparticle conductivity \(^\text{(4)}\) and of the CDW stiffness \(^\text{(10)}\). A detailed discussion of the effects induced by this convective term is beyond the scope of the present paper, therefore, we limit the discussion by a comment that some predictions of refs. \(^\text{4–6}\) must be revised.

Now we return to the transverse convective term. Its sign depends on the sign of the charge of the quasiparticles which determine the single-particle conductivity, and its temperature dependence is determined by an interplay of a thermally activated behavior and higher order terms in the interchain interaction. The exact value of the convective term depends on the details of the electron spectrum of the material. Using calculated values for the factors in equation of motion \(^\text{(7)}\) one can estimate the magnitude of the transverse electric field which may affect the CDW dynamics along the chains. In particular, following the calculations of ref. \(^\text{5}\) one gets a decrease of the threshold depinning field along the chains as a function of the perpendicular electric field \(E_\perp\) at \(E_\perp \gg E_c\), where \(E_c\) is the crossover field

\[
E_T(E_\perp) = E_T(0) \frac{E_\perp}{E_c} e^{2E_\perp/E_c}, \quad E_c = \frac{\sqrt{v_F E_T(0)}}{2 A v_\perp}. \tag{10}
\]

For the case of a semimetallic CDW material like NbSe\(_3\) when non-thermoactivated contribution to the factor \(A\) dominates, the crossover field can be estimated as

\[
E_c \approx \frac{\Delta^2}{t_\perp \mu v_\perp} \sqrt{E_\Delta E_T(0)}, \quad E_\Delta = \frac{\Delta^2}{v_F} \sim 10^4 \div 10^5 \text{V/cm}. \tag{11}
\]

The crossover field \(E_c\) is much larger than the longitudinal threshold field \(E_T(0)\) because both \(E_\Delta\) and the prefactor before the square root are large.

The experimental observation of the effect of a transverse current on the longitudinal CDW dynamics was reported recently by Markovic \textit{et al.}\(^\text{9}\) in NbSe\(_3\). It was found that application of a transverse electric field of the order of 1 V/cm was enough for a substantial reduction of the longitudinal threshold field. The discrepancy with the above estimate is thus 4-5 orders of magnitude. Now we discuss the problems which may occur in the experimental study of the effect in the simple geometry with two side contacts for the application of the transverse current\(^\text{9}\). Let us consider a sample of width \(w\) along \(y\) axis with side current contacts of length \(l\) along the \(x\) axis parallel to the chain direction. Assuming a uniform current density in the contacts and Ohmic conductivities \(\sigma_\parallel \gg \sigma_\perp\) in \(x\) and \(y\) directions (\(y = 0\) at the contact), respectively, we calculate the distribution of the electric potential in the sample (see ref. \(^\text{12}\))

\[
\phi = E_0 \frac{l}{2} \int_{-l/2}^{l/2} dx_1 \sum_{n=-\infty}^{\infty} \ln \sqrt{\frac{(x-x_1)^2 \sigma_\perp + (y+2nw)^2 \sigma_\parallel}{(x-x_1)^2 \sigma_\perp + (y-2nw)^2 \sigma_\parallel}}, \tag{11}
\]

where \(E_0 = j_\perp/(2\pi \sigma_\perp)\), \(j_\perp\) is the transverse current density through the contact.

In the case of large conductivity anisotropy, large components of the longitudinal current appear near the contacts. According to \(^\text{(11)}\) in the region near the contacts, at distances of the order of \(l\) along the chains and at distances about \(l \sqrt{\sigma_\parallel/\sigma_\perp}\) in the transverse direction,
the component of the electric field parallel to the chains is almost constant, \( E_\parallel \approx E_0 \). At larger distances the electric field decays as \( 2E_\parallel l/x \) at distances from \( x \gg l, y \sqrt{\sigma_\parallel/\sigma_\perp} \), and as \( 2E_\parallel x/y^2 \) at \( x, l \ll y \sqrt{\sigma_\parallel/\sigma_\perp} \). And, finally, it decays rapidly at \( x > w \sqrt{\sigma_\parallel/\sigma_\perp} \).

Thus, if a transverse voltage \( V \) applied to the sample is large enough, \( E_\parallel \) may be larger than the threshold depinning field \( E_T \). Moreover, the region where \( E_\parallel > E_T \) increases with increasing \( V \). Note also that the potential difference applied at different directions from the contacts along the chains is equal to \( V/2 \): the potential \( \phi \) decays along the \( x \) axis at distances of the order of \( w \sqrt{\sigma_\parallel/\sigma_\perp} \) from the contact (cf. Fig. 1). This voltage may easily exceed the threshold voltage needed to drive the CDW along the chains. In the experiments of ref. [9] \( l = 100 \mu m, w = 36 \mu m, \sigma_\perp/\sigma_\parallel \approx 0.04 \). Then for the characteristic value of the transverse current \( \sim 200 \mu A \) shown to suppress the longitudinal threshold field, we estimate \( E_\parallel \sim 0.3 \) V/cm. That is well enough for depinning the CDW for which \( E_T \approx 0.2 \) V/cm even if one takes into account the phase-slip voltage \( \sim 1 \) mV required for CDW breaking. So we conclude that the effect of the transverse electric field on the CDW dynamics can be easily masked by the CDW depinning by the longitudinal electric field component which is quite large due to large anisotropy of the conductivity. Moreover, when an additional longitudinal current \( I_{add} \) is applied to the central segment of the sample, the dependence of the threshold field on \( I_{add} \) mimics that of the transverse current observed in ref. [9] (see Fig. 1). It also shows the crossover current for the onset of the decrease of \( E_T(I_{add}) \) considered in ref. [8] as an argument against the possibility that the threshold field reduction is due to current inhomogeneities around the transverse contacts. The crossover behavior may be caused by the phase-slip voltage in the central segment where the currents \( I \) and \( I_{add} \) have the same direction (see inset in Fig. 1).

**FIG. 1.** Dependence of the threshold field of segment 2-6 on an additional longitudinal current in a geometry shown in inset for two samples of NbSe$_3$ with contact separations \( l_{23}, l_{34}, l_{45}, l_{56} \approx 100 \mu m \): \( \nabla - T = 115 \) K, \( \triangle - T = 128 \) . \( \circ \) and \( \bullet \) - dependence \( E_T(I_y)/E_T(0) \) on the transversal current \( I_y \) (data of ref. [9]). \( I_{add} \) is plotted in units \( I_T \) for our data, and \( I_y \) is multiplied by \( 6 \times 10^{-4} \) cm$^2$/A for data of ref. [9].

In conclusion, the calculated convective term is found to be much smaller than it was
originally suggested. Our analysis of the experimental verification of the effect shows that the observed behavior may be caused by geometric effects due to high anisotropy of the conductivity. So new experimental studies are needed.

We are grateful to N. Markovic and H. S. J. Van der Zant for detailed discussion of their work. This work has been supported by C.N.R.S. through the twinning program 19 between C.R.T.B.T. and IRE RAS, by the Russian Foundation for Basic Research (project 98-02-16667), and by Russian program “Physics of Solid State Nanostructures” (project 97-1052).
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