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Modeling of dislocations in a CDW junction: Interference of the CDW and normal carriers

Alvaro Rojo Bravo [a], Tianyou Yi [b], Natasha Kirova [c,d,*], Serguei Brazovskii [a,d]

[a] CNRS, LPTMS, URM 8502, Univeristé Paris-sud, Orsay 91405, France
[b] South University of Science and Technology of China, Shenzhen, Guangdong 518055, China
[c] CNRS, LPS, URM 8626, Univeristé Paris-sud, Orsay 91405, France
[d] International Institute of Physics, 59078-400 Natal, Rio Grande do Norte, Brazil

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ABSTRACT

We derive and study equations for dissipative transient processes in a constraint incommensurate charge density wave (CDW) with remnant pockets or a thermal population of normal carriers. The attention was paid to give the correct conservation of condensed and normal electrons, which was problematic at presence of moving dislocation cores if working within an intuitive Ginzburg–Landau like model. We performed a numeric modeling for stationary and transient states in a rectangular geometry when the voltage V or the normal current are applied across the conducting chains. We observe creation of an array of electronic vortices, the dislocations, at or close to the junction surface; their number increases stepwise with increasing V. The dislocation core strongly concentrates the normal carriers but the CDW phase distortions almost neutralize the total charge. At other regimes, the lines of the zero CDW amplitude flash across the sample working as phase slips. The studies were inspired by, and can be applied to experiments on mesa-junctions in $NbSe_3$ and TaS_3.

1. Introduction: CDW at a junction

It is supposed that in conventional junction and tunneling devices the applied voltage doesn't modify the electronic states, just only shifting their positions and fillings of bare ones. But in correlated systems, particularly with a spontaneous symmetry breaking, the electronic spectra are formed self-consistently via electron–electron or electron–lattice interactions. These effects can modify the ground state, the spectra and even the very nature of carriers and collective modes, which are transformed following changes in concentration of electrons near junctions. As a result, charge storage and a current conduction become different entities rather than the same electrons. These effects came to a broad attention only very recently with the goal of controlled phase transformations at surfaces by the electrostatic doping requiring for extreme strengths of the electric field [1].

The CDWs are particularly attractive because here the reconstruction of the junction takes place at moderate experimentally attainable electric fields. The problem came to attention first in theory [2,3], then in experiment [4], and it became a must in view of decisive experimental demands [5, 6] and in relation to other surface sensitive experiments [7,8]. The junction reconstruction in CDWs goes via appearance of topological defects (dislocations [9,10] as electronic vortices, as we shall call them below) with more microscopic solitons [11] as their cores.

We have already devoted studies and publications [12–14] to these problems. The numerical modeling was performed by the energy minimization for ground states under electrostatic voltage, by solutions of stationary PDEs for a system with running constant currents, solutions of time-dependent PDEs for transient processes recovering cascades of multiple vortices with a final stabilization for a few of them. While a kind of the Ginzburg–Landau (GL) or the time-dependent GL (TDGL) equations for the complex order parameter Ψ of the CDW was in the core of the model, they were greatly complicated in several aspects: the higher nonlinearity of the TDGL equation itself; coupling of Ψ with the normal carriers n which bring their own nonlinearity, retardations and dissipation via the diffusion equation; and particularly coupling to the electric potential Φ which brings the long range forces. This is the worst for the numerical work. Still, the simulations were always successful to an extent that they could be performed for realistic physical parameters and in actual sophisticated geometries of experiments.

* Corresponding author at: CNRS, UMR 8502 LPS, Univeristé Paris-sud 11, Bat. 510, 91405 Orsay Cedex, France.
E-mail address: kirova@lps.u-psud.fr (N. Kirova).

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Nevertheless, there is a serious demand for another, further complicated development which is described in this article and in [15]. In essence and by definition, the GL approach assumes integration over fermions (intrinsic carriers) participating in formation and distraction of the symmetry breaking, so that only Ψ is left explicitly. Even in statics, the GL equation can be derived for a small gap which takes place only near the transition line. Moreover, the TDGL equations, whatever for the superconductivity or for the CDW [16], can be derived only for a dirty metal when the scattering by impurities suppresses the quasi-particle gap completely (while still leaving alive the order parameter amplitude). This is not the regime which we are interested in and what is demanded by the experiment.

The question is not just about precising some qualitatively apparent forms and results. The partitions of the collective and the normal components in densities of the charge and the current change qualitatively, and that is particularly pronounced near the cores of moving vortices.

2. Anomalous equations and their interpretation

The CDW deformation $\sim\Delta\cos(Qx+\varphi)$ is described by the complex order parameter $\Psi=A\exp(i\varphi)$, $A=\Delta/\Delta_0$ where $2\Delta_0$ is the CDW gap at $T=0$. Two types of normal carriers may coexist with the CDW: the intrinsic carries $n_{in}=(n_e,n_h)$ (as electrons and holes above and below the gap) and extrinsic ones n_{ex}.

Extrinsic carriers do not participate in the CDW formation and they are coupled with the CDW only via the Coulomb potential Φ; their potential energy is $e\Phi$. These carriers belong to other electronic bands like pockets in $NbSe_3$ which example we shall imply. Their other sources can be non-gaped parts of an incompletely nested Fermi surface like in $TbTe_3$, etc. Intrinsic carriers exist in all realizations of, even if at low T they need to be activated across the gap. Their spectrum is formed by the CDW and their energies are displaced when the Fermi level E_F breathes up and down with expansions/contractions of φ. Their total potential energy

$$e\Phi+\frac{\hbar v_F}{2}\frac{\partial\varphi}{\partial x}$$

adds the coupling with CDW phase deformations. (From now on, we include the electronic charge e into the potential Φ, all energies and temperature are measured in units of Δ_0, the length will be still in nm.)

2.1. Equations

We start with the following form of the local energy functional (see [15] on hints of derivation)

$$W=\frac{\hbar v_F}{4\pi}\left[\left(\frac{\partial A}{\partial x}\right)^2+\beta^2\left(\frac{\partial A}{\partial y}\right)^2+\left(\frac{\partial\varphi}{\partial x}\right)^2+\beta^2A^2\left(\frac{\partial\varphi}{\partial y}\right)^2\right]+\frac{e}{\pi}\Phi\frac{\partial\varphi}{\partial x}+e\Phi n_{ex}+\left(e\Phi+\frac{\hbar v_F}{2}\frac{\partial\varphi}{\partial x}\right)n_{in}-\frac{\varepsilon s}{8\pi}(\nabla\Phi)^2 \tag{1}$$

We should add to that the local free energy of carriers $F_{ex}(n_{ex})+F_{in}(A,n_e,n_h)$. The dissipative evolution is described by Eqs. generated from the functional (1):

$$\frac{\partial}{\partial x}\left(\frac{\partial\varphi}{\partial x}+\frac{2}{\xi_0}\Phi+\pi(n_e-n_h)\right)+\beta^2\frac{\partial}{\partial y}\left(A^2\frac{\partial\varphi}{\partial y}\right)=\gamma_\varphi A^2\frac{\partial\varphi}{\partial t} \tag{2}$$

$$-\frac{\partial^2A}{\partial x^2}-\beta^2\frac{\partial^2A}{\partial y^2}+\beta^2A\left(\frac{\partial\varphi}{\partial y}\right)^2+\frac{\partial F}{\partial A}=-\gamma_A\frac{\partial A}{\partial t} \tag{3}$$

Here $\xi_0=\Delta_0/\hbar v_F$ and $\gamma_{A,\varphi}$ are the damping coefficients. γ_φ is related to the sliding CDW conductivity [12,13] which value fixes the time scale 10^{-13} s which will be the unit of our dimensionless time henceforth.

The Poisson equation for the electric potential is

$$\nabla^2\Phi=-\frac{\xi_0}{r_0^2}\left(\frac{\partial\varphi}{\partial x}+\pi(n_{in}+n_{ex})\right) \tag{4}$$

where r_0 is the Thomas-Fermi screening length of the parent metal and $n_{in}=n_e-n_h$.

The kinetics of normal carriers is taken in the quasi-equilibrium approximation.

$$\nabla(\sigma\nabla\mu)=\frac{e^2}{s}\frac{\partial n_{in}}{\partial t}\ ;\quad \mu=\zeta+\Phi+\frac{\hbar v_F}{2}\frac{\partial\varphi}{\partial x} \tag{5}$$

Here μ is the electrochemical potential $\zeta=\zeta(n,T)=\partial F/\partial n$ is the local chemical potential, $\sigma=(\sigma_x,\sigma_y)$ with $\sigma_i\sim(n_e+n_h)$ is the anisotropic conductivity tensor.

For boundary conditions, we assume that the normal CDW stress and the normal electric field are zero. The last arbitrary condition secures the total electro-neutrality and provides confinement of the electric potential within the sample which is convenient for calculations. The normal flow of the normal current exists only at two source/drain boundaries. As a whole, the boundary conditions have a form

$$\left(\frac{\partial\varphi}{\partial x}+\frac{2}{\xi_0}\Phi+\pi(n_e-n_h)\right)\nu_x+A^2\frac{\partial\varphi}{\partial y}\nu_y=0 \tag{6}$$

$$\nabla A\cdot\vec{\nu}=0\quad \nabla\Phi\cdot\vec{\nu}=0\quad \vec{\nu}\cdot\nabla\mu=0$$

Here $\vec{\nu}$ is the unit vector normal to the boundary.

The above Eqs. contain thermodynamic parameters: F and its derivatives. At a finite temperature T they can be calculated only numerically, so for the modeling we employed analytical interpolating formulas.

For F_{in} we used the BCS-Peierls form generalized to interpolate between small and large values of ζ.

$$F(A,\zeta)=A^2\left(\log\left(A^2+7\left(\zeta^2+T^2\right)\right)-1\right)\frac{2\pi}{\xi_0^2}$$

The minimum of $F(A,\zeta)$ at $A\neq0$ is erased (as it happens inside the vortex core) when ζ (hence n_{in}) is above a critical value. $n_e(\zeta,T)=n_h(-\zeta,T)$ were also given by formulas interpolating between large and small values of $|\zeta|$.

The dependence $\zeta(n)$ or $n(\zeta)$ defines dimensionless normal and collective particle densities:

$$\rho_n=\frac{1}{N_F}\frac{dn}{d\zeta}\ \text{and}\ \rho_c=1-\rho_n;\ N_F=\frac{2}{\pi\hbar v_F}$$

N_F is is the density of states of parent metal at E_F. In the metallic phase by definition $\rho_n=1$, then $\rho_c=0$, approaching from the CDW phase as $\rho_c\sim\Delta^2$.

2.2. Equations anomalies and their interpretation

Notice that the terms with $\partial_x\varphi$, $\partial_{xx}\varphi$ and $(\partial_x\varphi)^2$ in Eqs. (1), (2), (4) do not contain the usually supposed factor A^2. They are non-analytic in the order parameter Ψ and cannot be derived perturbatively; formally they appear because of the chiral anomaly [15].

Unlike the GL theory, all expressions containing $\partial_x\varphi$ are singular. Even the innocent Eq. (3) for A is not normal: A couples conventionally with $\partial_y\varphi$ but there is no complementary coupling with $\partial_x\varphi$ because there was no cross-term in the energy (1).

But taking all Eqs. in ensemble, we can notice, even if not explicitly, that the normal counterpart reacts negatively to variations of φ erasing the bare collective contribution in such a way that in terms with $\partial_x\varphi$ the factors 1 become $\rho_c=1-\rho_n$.