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LOCAL MECHANISM FOR GENERATION OF PERIODIC OSCILLATIONS BY MOVING CDW

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Abstract Generation of the quasiperiodic "noises" by moving CDW, as observed in a number of the Q1D metals, is ascribed to the boundary between the Peierls phase and an ordinary metal on which the CDW current is to convert into the normal one. The process is due to the periodically appearing phase slip centers where the local electron gap passes across zero. The simple microscopic model is suggested. Some possible regimes and the qualitative experimental consequences are discussed.

I. The bulk of the recent experiments in the inorganic Q1D metals of the $NbSe_3$-type is concentrated now in different aspects of the so-called "Frohlich conductivity mechanism" and the problem of the narrow band "noises" generated by the moving CDW[1-3]. The existing theories meet difficulties in attempts to explain the almost coherent character of the voltage oscillations generated in the sample by the current flowing in the presence of an electric field, E , exceeding the threshold field, E_t. It has been discovered experimentally[4,5] that the oscillations exhibit the local character and are probably connected with the vicinity of contacts (see the discussion in [6]). The phenomenological explanation suggested in [6,7] was based on the assumption that the effective electric field near contacts is substantially decreased (due to the better

contacts material conductivity) and this stops the CDW motion. The CDW "transport of phase" is compensated by the slippage of some phase vortexes The interpretation[7] was based on the phase hamiltonian using an analogy with the theory of the Josephson bridges.

Independently the author [8] has studied the phenomena occurring at the boundary between the Peierls state conductor and an ordinary metal, if in the Peierls material the current is partially due to the moving CDW. The main idea was to separate the impurity CDW pinning, which is the bulk effect, from the surface phenomena connected with a conversion of the CDW current into the normal carriers current at the border. The important comment is that any boundary creates some atomic displacements which are not sensitive to the low temperature structural transition in the Q1D metal. The Peierls deformation is to match the "tail" of these distortions introduced by the contact boundary. Therefore, the CDW is standing near the border. The crossover between this region and the distant region, where the CDW moves, takes place in a periodic phase slippage (PS) process, in which the dielectric "gap" (the CDW order parameter) locally passes across zero. This picture does not depend on the impurity pinning in the bulk and can be applied to any pure enough sample (low values of E_t). In addition, if at low fields the PS-centers are localized far apart from the boundary, its roughness will be smoothed out and will be unimportant for the nonlinear periodic regime. This could explain the approximately coherent character of the observed oscillations.

II The complexity of the electron spectrum of real

Q1D metals leaves no hope that a quantitative microscopic theory explaining all the experimental facts will be built up some time in future. Fortunately, the main properties of the CDW-type structural transition, as we understand now, can be described in simpler models, for instance, using the approximate relation for the electron spectrum

$$\varepsilon(p+Q) \simeq -\varepsilon(p) \qquad (1)$$

Here either $\underline{Q} = (2K_F, 0, 0)$ and Eq.(1) takes place owing to the quasionedimensional electron spectrum, or $\underline{Q}$ equals $(2K_F, 1/2; 1/2)$, as in the tight binding model for which Eq.(1) would be exact [9]. The Peierls transition acquires the thermodynamic sense either due to 3D phonons, or owing to the finite transverse electron dispersion (the latter is probably correct at least for $NbSe_3$). On the other hand, for the Frohlich mechanism to occur it is only necessary that the Q-vector in Eq.(1) would have an incommensurate component $2K_F$ along the main conducting axis. For this the Fermi surface is to consist of a few open sheets lying near $\pm K_F$ planes in the zone. In such a model the microscopic theory with the well defined applicability criterion can be formulated. The most simple equations for the order parameter $\Delta = |\Delta| \exp(i\varphi)$ (as usual, Δ is proprotional to the lattice deformation) have been obtained [8,10] in the so-called "gapless limit" when impurities almost suppress the structural transitions.

These equations are of the form;

$$\dot{\Delta} + iE_x\Delta - \Delta + |\Delta|^2\Delta - \nabla^2\Delta = 0 \qquad (2)$$

and the expression for the electric current is

$$j = E - \lambda E|\Delta|^2 - \bar{\lambda}|\Delta|^2\dot{\varphi} \qquad (3)$$

Eqs. (2,3) already contain dimensionless variables. Their explicit definition can be found in [10,11]. In Eq. (3) $\lambda, \bar{\lambda} \ll 1$ and this reflects the fact that in the "gapless limit" ($\tau T_p \ll 1$) the current is mainly carried by the normal carriers. This substantially simplifies Eq. (2), because in the first approximation the electric field E_x is fixed by the current. The voltage oscillations obliged to the PS-centers do appear as small corrections in Eq. (3). The real space scale in Eqs. (2,3) is $\xi_0 \sim \hbar v/T_p$ and the electric field is measured as $eE\xi_0/T_p$.

III. Eq. (2) suggests probably the most simple microscopic model for the study of the nonlinear periodic regime with the PS-centers at the boundary. On the left (i e, at $x \to \infty$) $\Delta = \exp(-iEt)$ and this solution describes the moving CDW. Taking Δ fixed at $x = 0$ ($\Delta_0 = 1$ for simplicity, see below), near the boundary one would get the static solution:

$$|\Delta|^2 = 1 - Q^2 \; ; \; 3Q - Arth\, Q = Ex \qquad (4)$$

(here $Q = \nabla\varphi/\partial x$). According to (4), Q increases with $|x|$, while $|\Delta|^2$ decreases. A finite $Q = \nabla\varphi \neq 0$ merely means a local change of the nesting vector, or some deviations from the optimal nesting conditions Therefore, the static solution (4) is only stable at $|x|$ smaller than some x_0. Near x_0 the exact solution of Eq. (2) becomes essentially time-dependent and $|\Delta|$ periodically passes across zero This results in the phase loss $[\varphi] = 2\pi$ at each such an event.

The form of static solution (4) shows that x_0 could be large for a weak enough field (if $E \ll 1$, $Q \sim 1$ at $x \sim E^{-1}$) However, the complex function $\Delta(x,t)$ is described by the nonlinear Eq.(2) and the point x_0, where the regime (4) becomes unstable, can be found only from its straightforward integration. It is important to emphasize that each PS-center has the dynamic struture (the regime represents a cycle). In fact, let us assume that tat some x_0 $\Delta(x_0, t = 0)$. Being linearized in Δ, Eq (2) belongs to the parabolic type. Using the standard diffusion solution, one easily shows that for the subsequent time moments, $t > 0$, $\Delta(x_0, t) \neq 0$.

The numerical calculations [11] gave $x_0 \simeq 1.15\, E^{-0.28}$ ($E \ll 1$) and this is not very sensitive to the choice of $\Delta_0 \neq 1$ Thus, while the PS-position, x_0, exceeds the coherence length ($\xi_0 \sim 10^{-6}$cm), the growth of x_0 with the field decrease is comparatively slow. In this connection it is relevant to discuss again the boundary conditions for Eq.(2). Deformation, induced on the contact, is large and the solution is to reflect this fact. Near the boundary the three first terms in Eq.(2) can be omitted ($\Delta \gg 1$). The first integral has the form:

$$|\Delta|^2 Q = q; \quad (|\Delta|')^2 - \frac{|\Delta|^4}{2} - \frac{q^2}{|\Delta|^2} = c_1 \qquad (5)$$

The integration constants, q and c_1, are defined by the bulk solution. The demand that $|\Delta|$ have a growing behaviour at $x \to 0$ would give the rigorous boundary conditions in the form:

$$|\Delta(x)| = (\sqrt{2}\, x)^{-1}; \quad Q = \partial\varphi/\partial x = 2qx^2 \sim 0; \quad \text{at} \quad x \to 0 \qquad (6)$$

So far Eqs(6) have never been used in numerical calculations.

IV. The idea that near contacts the CDW is fixed, makes possible the formulation of the threshold field problem for the sample of a finite length, L. If L is small, the CDW motion in the internal part of the sample will start in a strong enough electric field. The numerical result [11] for $E_t(L)$ is

$$E_t(L) \simeq 2.25\ L^{-1.23}$$

This motion introduces the phase slippage inside the sample or near its two ends. The generation of oscil - lations and details of the nonlinear regime can be studied in good quality samples and are not dependent on the impurity pinning.

V. In the above and in [11] the slippage at which $\Delta(x,t)$ gets zero homogeneously across the whole sample, have been considered. Obviously, such a solution is applicable only for a thin enough sample. If the transverse sample sizes are large, the different regime would be possible. In this case the slippage is due to the transverse motion of the chain of dislocations in the Peierls superlattice. Each separate dislocation is to compensate the phase growth $[\varphi] = 2\pi$ at its motion across the sample. Their linear density is therefore defined by the CDW current far from the boundary. No numerical calculation have been so far done for this much more complicated regime.

Microscopic Eq.(2) of course oversimplifies substantially the situation: in the real material the anisotropy (or "the one-dimensionality") is important. The main difficulty connected with 1D features lies in a more appropriate account of the energy and momentum relaxation between different excitations and between excitations (electrons and phonons) and the "conden-

sate". The corresponding equations can be written down again for the simple model of Eq.(1), however, this time they would be too complicated even for the numerical approach. The most important new fact is that the time evolution of the phase is characterized by two different scales.

In conclusion, we have shown that the conversion of the CDW current into a current of the ordinary electrons near the boundary surface take place in the nonlinear time-periodic regime of the order parameter variation. The regime corresponds to discontinuous jumps of the phase while the magnitude of the local CDW gap passes across zero Unlike the approach with the phase hamiltonian or various soliton models, the suggested picture does not lead to any difficulties with the charge accumulation either.

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