Multi-fluid hydrodynamics in charge density waves with collective, electronic, and solitonic densities and currents.

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Collaboration: Natasha Kirova, LPS, Orsay, France, 1999&2019
Serguei Matveenko 1989

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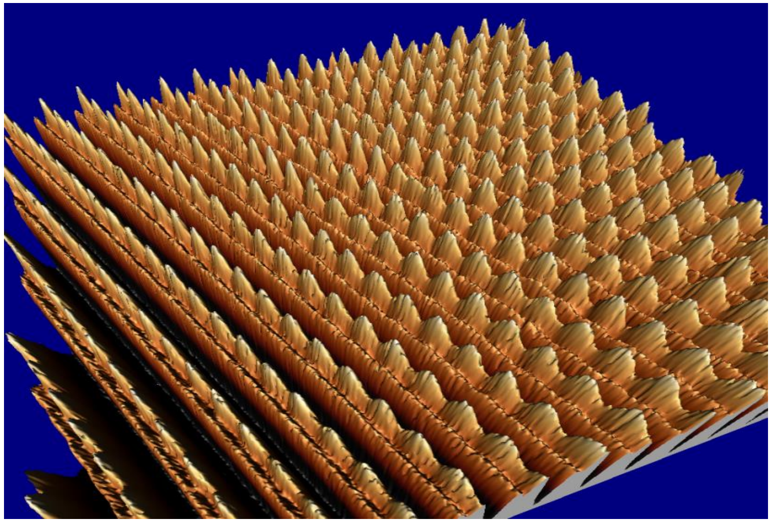
JETP, I.M. Khalatnikov anniversary volume, 2019

Scanning Tunneling Microscopy STM shows the CDW modulation in atomic displacements and the electronic density.
Brun, Wang, Monceau, SB



Main features of electronic crystals like Wigner crystals, charge density waves CDW, etc.

- Space periodicity follows a local concentration of condensed electrons
- Collective sliding under a driving field above the threshold E_t.
- Collective sliding is a periodic coherent anharmonic process.
- Excess normal current is converted to the collective one via phase slip processes.
- Transverse flow of dislocations is an ingredient of sliding and of current conversion.
- Point defects – solitons as vacancies/addatoms are favorable in comparison with electrons as normal carriers.
- Energetics of dislocation lines/loops is determined by Coulomb forces and by screening facilities of the free carriers.

atomic density ρ_{atomic}	modulation $A\cos(Qx+\varphi)$
displacements $\vec{u}/a$	$-\vec{\nu}\varphi/2\pi$, $\vec{\nu}=(1,0,0)$
compression $-\nabla\vec{u}$	charge $\partial_x\varphi/\pi$
velocity $\partial_t\vec{u}$	current $-\vec{\nu}\partial_t\varphi/\pi$
vacancies or addatoms	$\mp 2\pi$ solitons
dislocations	phase vortices

Dislocation in CDW versus vortex in SC

$$\Psi_{CDW} = A\exp(i\varphi)$$

$$\Psi_{SC} = C\exp(i\theta)$$

$$j_{CDW} = -A^2 \frac{e}{\pi}\frac{\partial\varphi}{\partial t}$$

$$n_{CDW} = A^2 \frac{e}{\pi}\frac{\partial\varphi}{\partial x}$$

$$j_{SC} \propto C^2 e v_F \frac{\partial\theta}{\partial x}$$

$$n_{SC} \propto -C^2 \frac{e}{v_F}\frac{\partial\theta}{\partial t}$$

Equivalence of actions of **E_y** and **H_z** upon the order parameters.

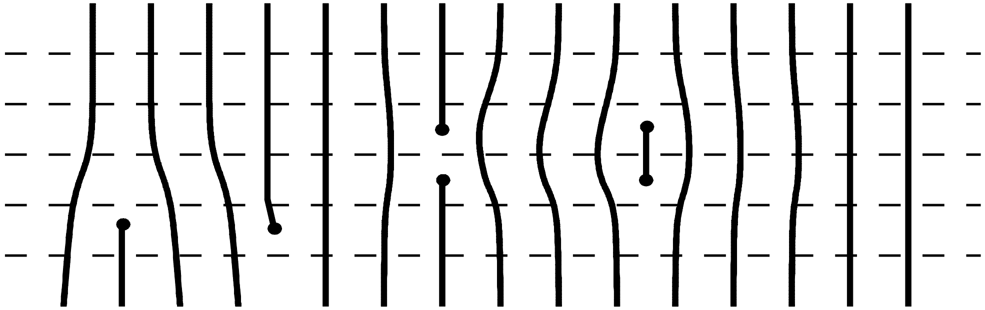
Reverse effect of order parameters upon the fields are opposite:

CDW – transverse electric field **E_y** is screened only via dislocations.

SC - magnetic field enters via vortices.

Unlike **H≈cnst** in SC, **E** in CDW is always strong,
needs to be determined self-consistently

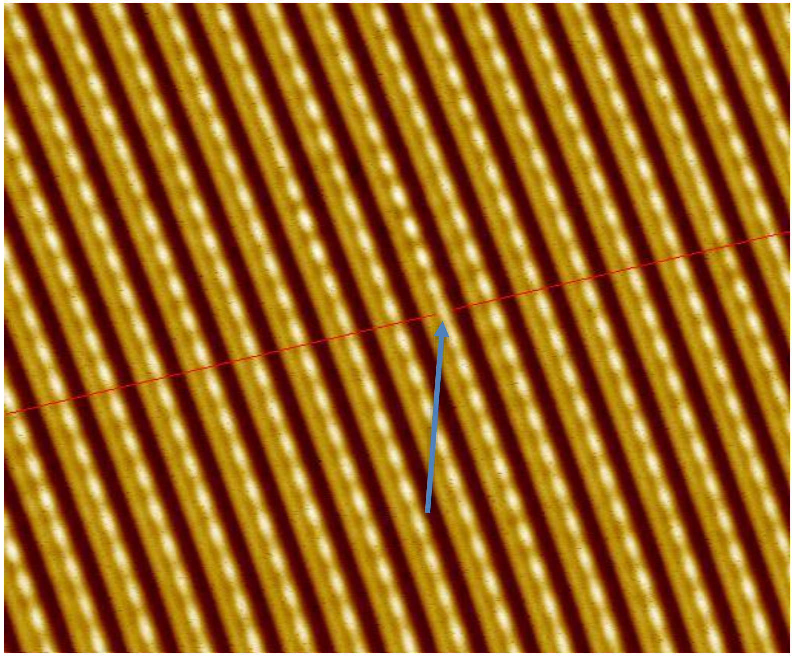
Topological defects in a CDW: dislocations, their pairs, the soliton.



dislocations *and* their pairs

Solid lines: maxima of the charge density.

Dashed lines: chains of the host crystal.



By passing each of these defects, the phase changes by $\mathbf{2\pi}$.

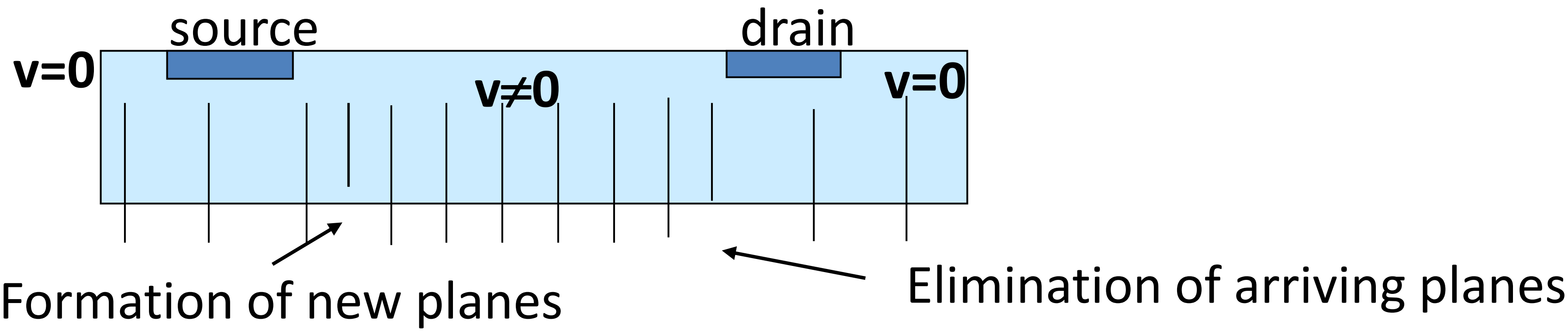
Embracing only one chain of atoms, the pair become a vacancy or an interstitial $\Rightarrow \pm 2\pi$ solitons in CDW

STM image of CDW chains with one defect as $\mathbf{2\pi}$ solitons.

At the (red) front line the defected chain is displaced by half of period.

Along the defected chain the whole period $\pm\mathbf{2\pi}$ is missed or gained

Dynamic origin of dislocations



To set up CDW motion with a velocities **v**:

Transfers flow of vortices - thick channel *(Maki&Ong)*

Coherent phase slip - thin cannel (Gor'kov)

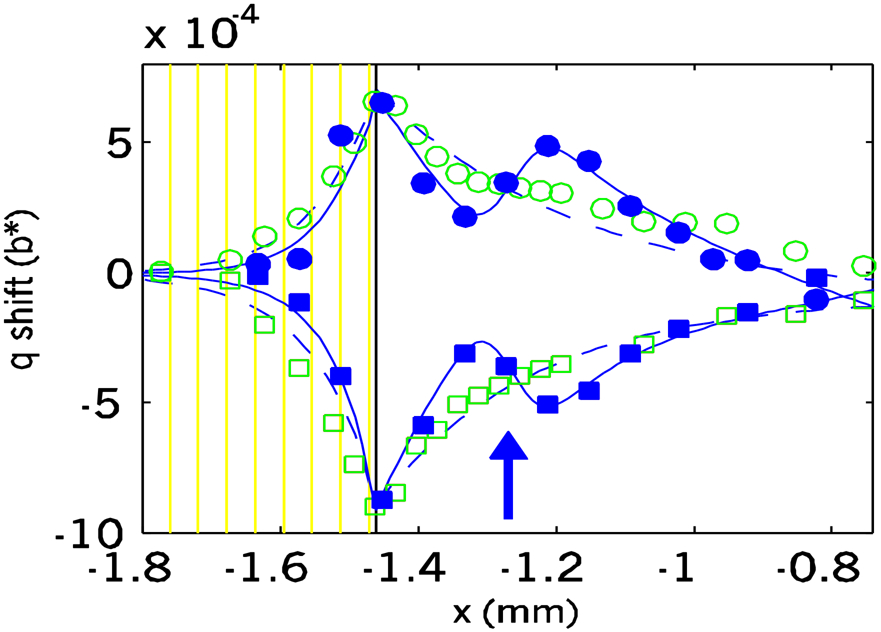
Phase slips:

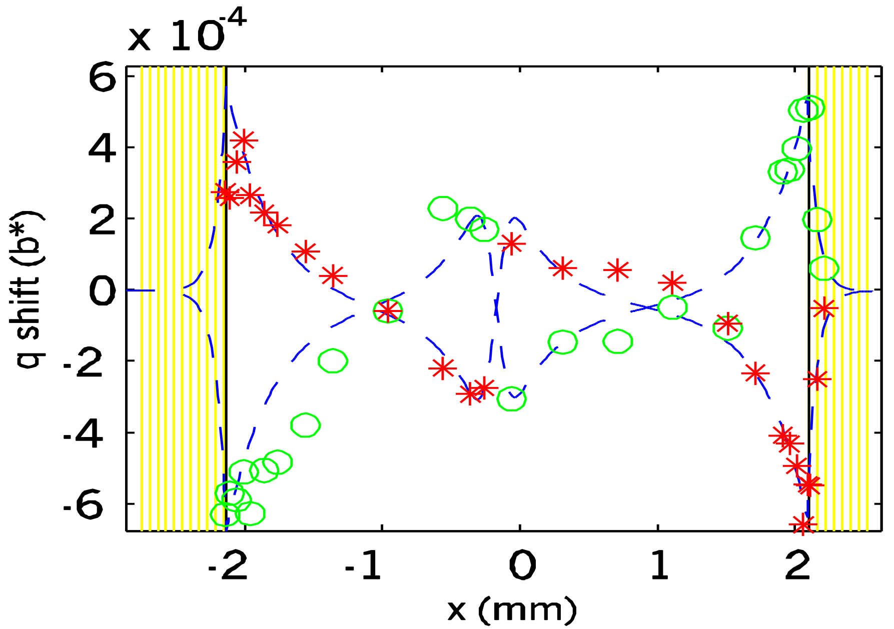
Microscopically **–** self-trapping of electrons into solitons, their subsequent aggregation.

Macroscopically – the edge dislocation line proliferating/expanding across the sample.

Pinning and plasticity at macroscopic scales.
CDW flow throw a crossection with an enhanced pinning force

Measuring local strain ***q*= ∂ϕ/∂x** via space resolved X-ray diffraction
Rideau, SB .. et al 2001. *Lines – theory fits after SB & N.Kirova*.

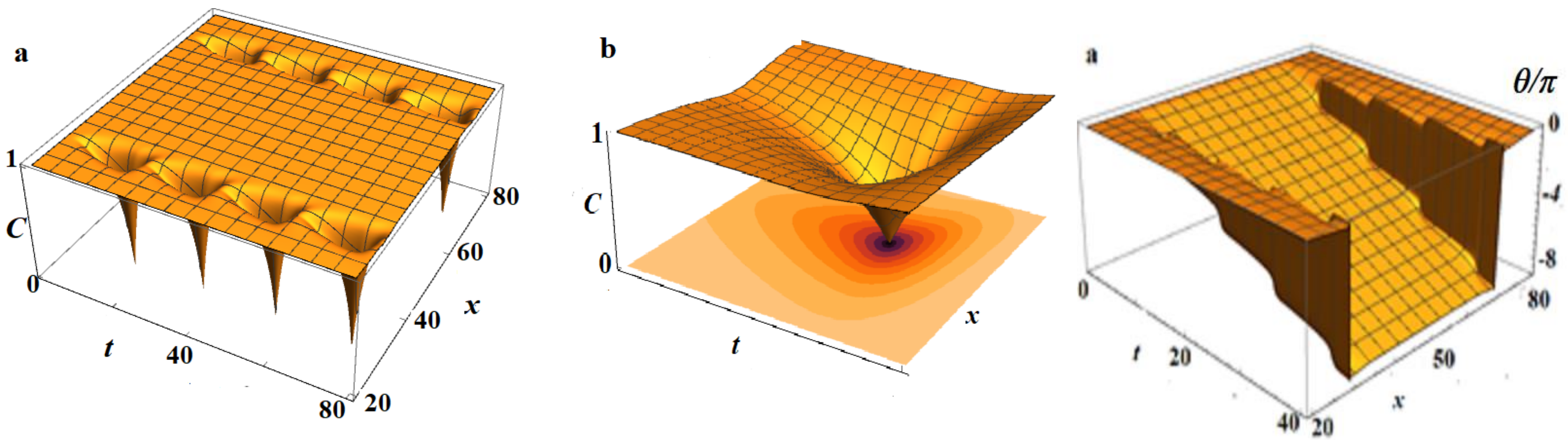




A fabricated region of smoothly increasing friction:
The stress is built up to help the CDW to pass by intact.

Sharp strong obstacle near **x=0**.
Crossing curves for opposite **J** signifies a partial (re)conversion by phase slips – flashing dislocations.

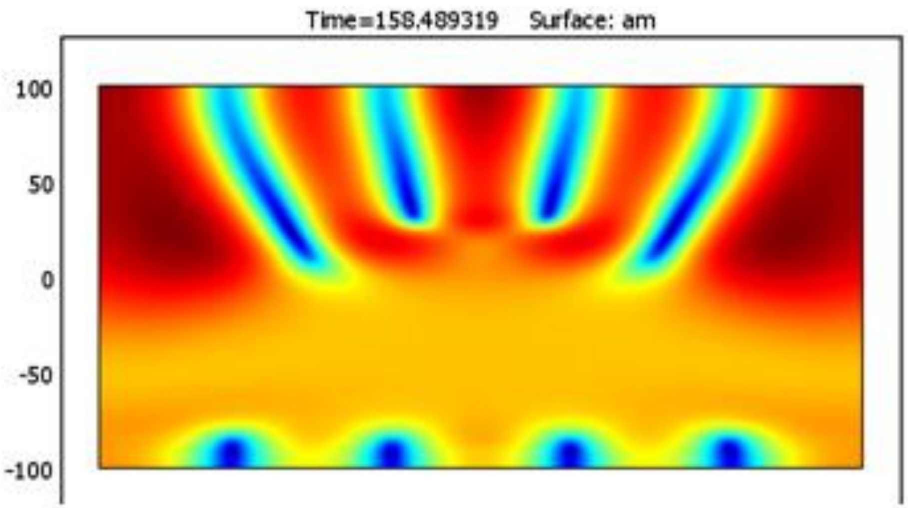
Numerical modeling of a spontaneous sequence of phase-slips = space-time vortices

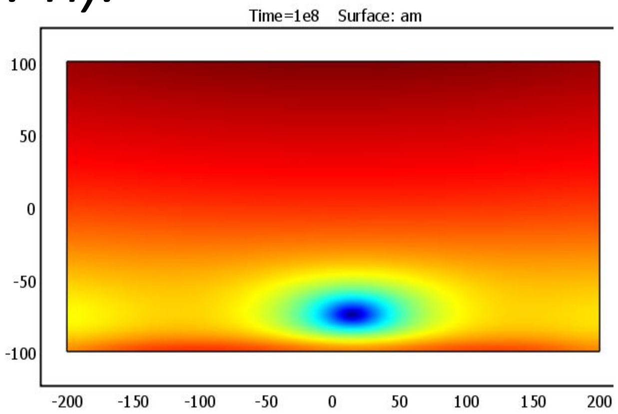


SB & N. Kirova, 2019

Sample reconstruction by applying the transverce voltage to adopt the first stable vortex – analoge of Hc1 in superconductors.

Many temporary vortices appear in the course of the evolution.
GL based modeling *(SB, N. Kirova and T. Yi).*



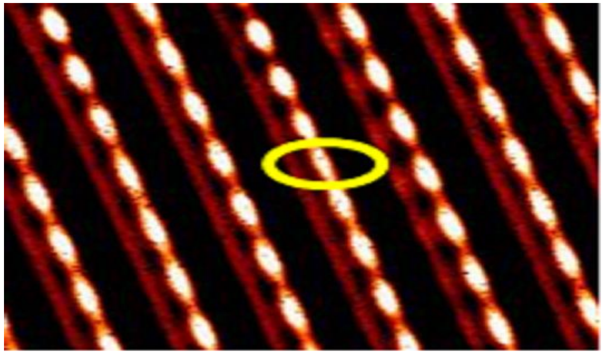


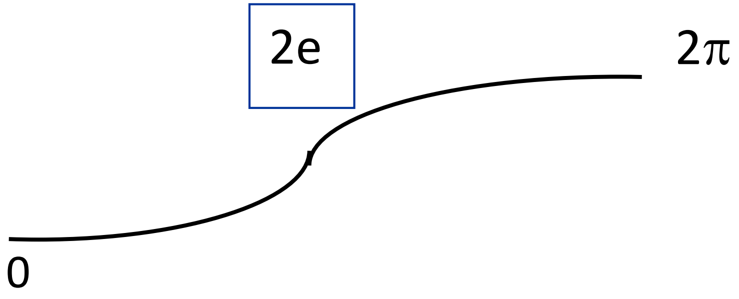
The single stable vortex is left: analog of **Hc1** in SC

Long living traces of amplitude nodes following fleshes of vortices.

Phase deformations cannot relax fast following rapidly moving vortices

Phase solitons (PhS): significance, contradictions, motivation.





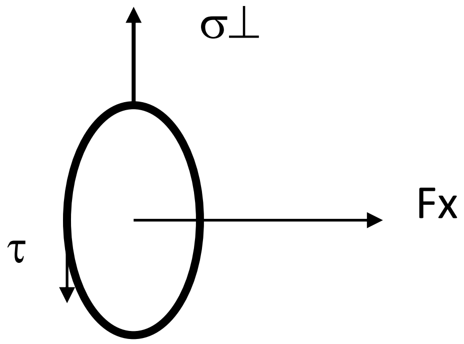
1. PhSs are main observable "single-particle" carriers of on-chain || currents with activation energies $\sim T_c \ll \Delta$ for electrons which are seen in ⊥ transport .

2. As **2e** charges localized over $\hbar v_F/T_c$ they must create a local electric field and carry a local current;

3. Like electrons, or vacancies/addatoms, they seem to carry a mean current being driven by the mean electric field which is wrong:

4. Being pairs/loops of dislocations they produce long range tails which exactly compensate charges, currents, forces in average over any cross-section. Particles' currents are transferred to collective mode.

5. Even the local force $\mathbf{F_x}$ ≠ the gradient of their potential energy **U** under the local stress $\boldsymbol{\sigma}$:



$$F_x \sim \oint \vec{\sigma} \times d\vec{l} \neq -\partial_x \iint \vec{\sigma} d\vec{s} = -\partial_x U \Leftarrow \nabla \vec{\sigma} = F_{friction} \sim \partial_t \varphi \neq 0$$

Kinematics at presence of dislocation lines/loops (DL)

Local deformations and velocities are not derivatives of a same phase

$$\frac{\partial \phi}{\partial t} \rightarrow \omega_t \,,\; \frac{\partial \phi}{\partial x} \rightarrow \omega_x \,,\; \frac{\partial \phi}{\partial y} \rightarrow \omega_y \,,\; \frac{\partial \phi}{\partial z} \rightarrow \omega_z$$

Four variables: $(\omega_x\, \omega_y\, \omega_z\, \omega_t)$ instead of one φ

$(\omega_x\, \omega_y\, \omega_z) = \omega$

$$\omega \neq \nabla\varphi \leftrightarrow \nabla\times\omega \neq 0$$

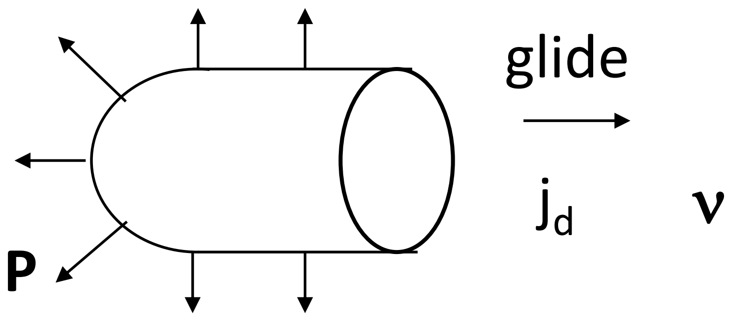
$$\vec{\tau} = \frac{1}{2\pi}[\nabla \times \vec{\omega}]$$ - density of DLs, space circulation of φ

$$I = \frac{1}{2\pi}(\nabla \omega_t - \frac{\partial \omega}{\partial t})$$ - flow of DLs, space-time circulation of φ

Phase circulation

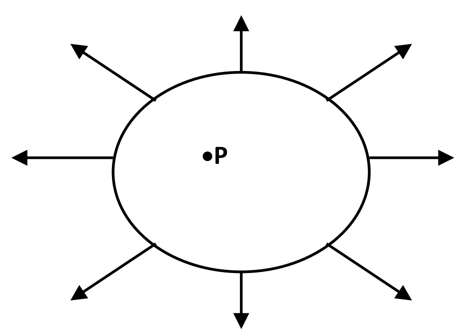
Two types of dislocation motion: Glide and Climb

Glide - conservative motion of DLs along the Bourges vector || chains' direction



Climb: transverse motion of D-lines or growth/shrinking of D-loops by *adhesion of non-crystalline matter = conversion of electrons in CDWs*.
$dn_d/dt \neq 0$, n_d – density of defects = transverse area of D-loops.

$$F_\perp \propto \int T_x dl$$



Expansion
= climb

Invariant averaging over D-loops, including solitons

n_d – density of defects = projected DL area per volume $\frac{dn_d}{dt} = -2\frac{dn_n}{dt}$

Averaging result:

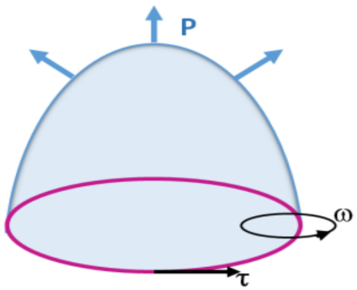
$$\langle \vec{\tau} \rangle = -[\vec{\nu}\vec{\nabla}]n_d \qquad \langle [\vec{\nu}\vec{\tau}] \rangle = -\vec{\nabla}_{\perp} n_d \qquad \langle I \rangle = \vec{\nu}\frac{\partial n_d}{\partial t} + \vec{\nabla} j_d$$

Consequences:

There is a uniquely defined function χ such that

$$\partial_t \chi = \langle \omega_t \rangle / 2\pi + j_d \qquad \partial_x \chi = \langle \omega_x \rangle / 2\pi + n_d \qquad \partial_{y,z} \chi = \langle \omega_{y,z} \rangle / 2\pi$$

Invariantly averaged phase χ reduces four equations for four variables ω_i to the single one, as it was without vorticity.



P – density of discontinuities at arbitrary surfaces based on DL:

$$\omega + 2\pi \mathbf{P} = \nabla\varphi \qquad \tau = -\left[\nabla \times P\right] \qquad I = \frac{1}{2\pi}(\nabla\omega_t - \frac{\partial\omega}{\partial t}) + \frac{\partial\vec{P}}{\partial t}$$

τ,I - physical singularities at the DL,
P, φ – non-physical singularity at a surface based upon the DL

Fix the time dependent part of the gauge:

$$\omega_t = \frac{\partial\phi}{\partial t} \quad \Rightarrow \vec{\nabla}\omega_t = \frac{\partial}{\partial t}\left(\vec{\omega} + 2\pi\vec{P}\right) \quad \Rightarrow \vec{I} = 2\pi\frac{\partial\vec{P}}{\partial t}$$

ω_l, I are singular at DL only. Now the same holds for $\partial_t\vec{P}$
Discontinuity surface $\vec{P}$ is arbitrary only at some initial t=0.
Afterwards $\vec{P}$ evolves only along the surface passed by DL, that is following the trace of physical singularities.

From kinematics to dynamics.

Local material relations:

Velocity : $\mathbf{v=\varphi_t} \leftarrow \partial\varphi/dt$

Strain : $\omega \leftarrow \nabla\varphi$ Stress : $\sigma = \delta W/\delta\omega$

Equilibrium:

$\nabla\sigma = F_{frc}(v) \leftarrow m\,dv/dt + \gamma v$

Defect energy per chain $\sigma_x = U$

Force driving current of defects is NOT the gradient of their potential:

$F_{dx} \neq -\partial_x U$ but $$F_{dx} = \hat{\Delta}_{\perp}\chi$$

The two forms are not identical because $\nabla\sigma = \text{friction} \neq 0$

Glide of defects is enforced by share strains - gradients transverse to chains.

DW specific relations:

Poisson equation: $\delta W/\delta\Phi = 0$

Normal carriers:

Chemical potential : $\zeta_n = \delta W/\delta n$

Current: $j_n = -\sigma_n \nabla\mu$

Conservation :

$$\frac{\partial n_n}{\partial t} + \nabla j_n = \frac{dn_n}{dt}$$

Source – drain = conversion

$$R(\mu_d - \mu_n) = \frac{dn_d}{dt} = -2\frac{dn_n}{dt}$$

n_n – normal electrons

R phase slip rate= conversion rate

R(0)=0 – important and ambiguous physical input

The CDWs functional of the free energy W
(linear density per chain area):

$$W = \frac{\hbar v_F}{4\pi}\left[\omega_x^2 + \alpha_y \omega_y^2 + \alpha_z \omega_z^2\right] + \frac{e}{\pi}\omega_x \Phi$$
$$+\left(e\Phi + \frac{1}{2}\hbar v_F \omega_x\right) n_n + F_{loc}\left(n_n, A\right) - \frac{1}{8\pi}\left(\nabla\Phi\right)^2$$

A – CDW amplitude, the gap Δ**~A**

$\alpha_{x,y}$ ~A^2 - share modules from interchain CDW coupling

n_n – concentration of normal carriers

$F_{loc}(n_n, A)$ - free energy at a given concentration of normal carriers.

The local balance of forces for the viscous media

$$\vec{\nabla}\vec{\sigma} = F_{frc} \Rightarrow F_{pin} + \frac{\gamma}{\pi}\partial_t \varphi; \quad \vec{\sigma} = \pi \frac{\delta W}{\delta \vec{\omega}}$$

The stress:

$$\sigma_x = \frac{\omega_x}{\pi} + \Phi + n_i; \quad \sigma_y = \frac{\alpha_y \omega_y}{\pi}; \quad \sigma_z = \frac{\alpha_z \omega_z}{\pi}$$

The Poisson equation:

$$r_0^2 \Delta\Phi + n_0 + n_i + n_e + \omega_x / \pi = 0 \qquad r_0^{-2} = \frac{8e^2}{s\hbar v_F}$$

Equations for average variables

$$\left(\partial_x^2 + \alpha\Delta_\perp^2 - \gamma\partial_t\right)\chi = -\partial_x\Phi - 2\gamma j_d - \partial_x\left(n_n + 2n_d\right)$$

$$r_0^2\Delta\Phi + \partial_x\chi = -\left(n_n + 2n_d\right)$$

$$n_{tot} = \omega_x/\pi + n_n = \partial_x\chi + 2n_d + n_n \text{ then } \vec{j}_{tot} = (-\partial_t\chi + 2j_d)\vec{\nu} + \vec{j}_n$$

The density and the current of defects contribute
in the frame of the average phase χ
while they were doomed with respect to local deformation **ω**

What does drive the phase: friction of D-loops,
|| gradient of their concentration together with normal carriers

At presence of noncompensated dislocation lines

$$[\vec{\nu}\vec{\nabla}][\left(\hat{\Delta} - \gamma\partial_t\right)\chi + 2\gamma j_d + \partial_x(n_i + 2n_d) - F_{pin} - E] = 2\partial_x\vec{\tau}_D$$

Conservation law for the total charge

$$\frac{dn_d}{dt} = -2\,\frac{dn_n}{dt} = R \qquad \frac{dn_a}{dt} = \frac{\partial n_a}{\partial t} + \vec{\nabla}\,\vec{j_a}$$

$$a = n, d \qquad \vec{j_d} = \vec{v}\, j_d$$

R(δμ) – conversion rate. Currents of normal carriers:

$$\vec{j_a} = -G_a \nabla \mu_a; \quad \mu_a = \frac{\delta W}{\delta n_a} = V_a + \varsigma_a\,, \quad \varsigma_a = \frac{\delta W_{loc}}{\delta n_a}$$

$$V_e = \Phi, \quad V_i = V$$

$$-\partial_x V_d \Rightarrow 2\hat{\Delta}_\perp \chi \neq -\partial_x V_d\;,\; j_d = -2G_d(\hat{\Delta}_\perp \chi + \partial_x \zeta_d)$$

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$\mathbf{n_{\pm}}$ - the partial concentrations of defects with two signs of vorticity,
$\mathbf{n_{+}}$ - $\mathbf{n_{-}}$ =$\mathbf{n_{d-}}$ – sign-sensitive mean concentration of defects,
$\mathbf{n_{+}}$ + $\mathbf{n_{-}}$ =$\mathbf{n_{d+}}$ – total concentration of defects of both signes,
In equilibrium chemical potential $\boldsymbol{\zeta_d}$**=0** , $\mathbf{n_{d+}}$ **=** $\mathbf{n_{d,tot}}$
Forces: $\pm\mathbf{F_d}=\pm\Delta_{\perp}\chi$. Currents of defects in the diffusion approximation,

$$j_d = b_d F_d (n_+ + n_-) - D_d \partial_x (n_+ - n_-) = b_d n_{d,tot} (\hat{\Delta}_\perp \chi - \partial_x \zeta_d)$$

$$n_\pm = n_\infty / 2 \exp\left(\pm \zeta_d / T\right)$$

$$\left(\hat{\Delta} - \gamma \partial_t\right) \chi + 2\gamma b_d n_{d+} \Delta_\perp \chi + 2(\gamma D_d + 1) \partial_x n_{d-} = E + F_{pin}$$

the allowance for defects' motion contributes additively to the $\Delta_\perp \chi$ transverse rigidity of the phase and to the driving force from the gradient of the defects' concentration

CDW reality: unscreened Coulomb forces, low temperature

Nonlocality of Coulomb interactions: nonlocal elasticity, higher order of the Laplassian

r_0 –Debye screening length in a parent metal.

Resulting phase equation:

$$\left[r_0^2 \Delta_\perp \left(\Delta_\perp - \gamma \frac{\partial}{\partial t} \right) - \frac{\partial^2}{\partial x^2} \right] \chi = \frac{\partial}{\partial x} \left(n_n + 2 n_d \right) + 2 \gamma j_d$$

Electroneutrality at $r_0=0$

Driving force:
only || gradients of normal carriers and defects

Crosssection integration at at r_0=0 :

Gapful CDW at low T, the only carriers are the phase solitons.
The specific driving force $\Delta_\perp \chi$ upon defects vanishes after the integration in view of the zero-stress side boundary conditions.
The integrated current of defects is driven only by the diffusion:

$$\partial_x \overline{\chi} + 2\overline{n}_d = 0 \; , \; \partial_t \overline{\chi} + 2D_d \partial_x n_d = -J(t) \; ,$$

$$(D_d \partial_x^2 - \partial_t)\overline{\chi} = J(t) = E / \gamma$$

These simple relations show actually not always expected results:

1. Solitons do add to charge density and current on top of collective ones.
2. The elastic response $\partial_x^2\chi$ to the current **J** is given curiously by the diffusion coefficients of defects.
3. The elastic response $\partial_x^2\chi$ to the electric field **E** contains the product γD_d of kinetic coefficients: collective mode friction and the diffusion of its nonlinear excitations. The conventional thermodynamic elasticity (**$E=\partial_x^2\chi$**) is suppressed by the electroneutrality condition **r_0=0**.
4. The **I-V J(E)** dependence does not know about defects: all goes to the indistinguishable sliding.

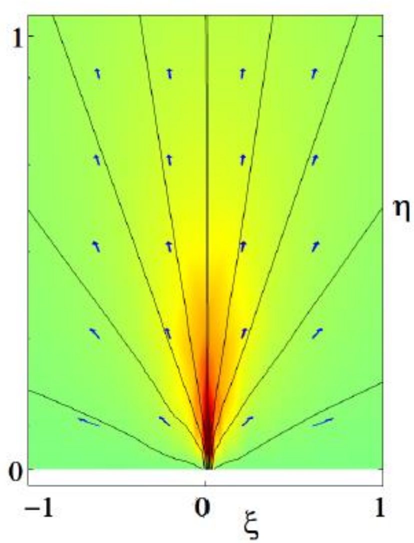
Isolated dislocation at presence of solitons.

$$[r_0^2\alpha_y\partial_y^4-\partial_x^2]\chi-\partial_x(n_n+2n_d)=\partial_x\delta(x)\mathrm{Sgn}(y)$$

$$-\partial_x\Phi=\alpha_y\partial_y^2\chi$$

$$n=n_\infty\sinh\frac{\zeta}{T} \qquad l_{scr}=r_0\left(\frac{T}{2n_\infty}\right)^{1/2}$$

$$2n_\infty\left(l_{scr}^2\partial_y^2\frac{\zeta}{T}-\sinh\frac{\zeta}{T}\right)-\partial_x\chi=0\ ,\ \partial_x\zeta=\Phi=\alpha\partial_y^2\chi$$



Distributions around a dislocation centered at (0,0);
Vectors and streamlines characterize the phase.
The color indicates the chemical potential zT.
Z changes from 0 at large distances (green color) to a maximal value 2.5 (abundance of solitons) near the origin (red) and then drops to zero (blue).

Local energy functional

$$\psi = A\exp(i\varphi) \qquad A=\Delta/\Delta_0$$

$$\varphi_i = \partial\varphi / \partial x_i$$

$$W\{\varphi,\Phi,n_n,A\} = \frac{\hbar v_F}{4\pi}\left[\varphi_x^2 + \alpha A^2 \varphi_y^2\right] + \frac{1}{\pi}\varphi_x \Phi + \left(\Phi + \frac{\hbar v_F}{2}\varphi_x\right) n_n + F(A, n_n)$$

Expect A^2 – actually 1.
Non analytic in Ψ

Both terms are **not** derivable perturbatively – the chiral anomaly.

$F(A,n_n)$ - free energy of vacuum and normal carriers

$$n = \frac{1}{\pi}\partial_x \varphi + n_n \ , \qquad j = -\frac{1}{\pi}\partial_t \varphi + j_n \Rightarrow \frac{dn}{dt} = 0$$

An implicit mechanism for $\boldsymbol{n_n}$, $\boldsymbol{j_n}$ to compensate $\boldsymbol{\partial\varphi}$ at $\boldsymbol{A\to 0}$

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Conclusions

The presented scheme is a minimal version of the multi-fluid hydrodynamics of plastic flows in CDWs. The results:

- provide phenomenologically rigorous relations among observables
- allow for some, not quite expected, interpretations, particularly on the control variables and driving forces
- provide a basis for analysis of modern experimental studies of CDW at constraint geometries, meso & nano scales.
- Theory still needs to take into account the distribution, and its evolution, of loops' dimensions to describe their aggregation towards macroscopic objects.