Expanding observations of solitons in quasi one-dimensional conductors. Routes to a role of microscopic topological defects in general strongly correlated electronic systems - repulsive and attractive.

Motivation: What Charge Density Waves can tell to: Doped Mott Insulators, Spin-Polarized Superconductors, etc. From solitons in 1D models to solitonic lattices, stripes and FFLO state, and back to combined topological excitations with spin-charge reconfinement.

Sources: Joint work with experimental groups of
Grenoble (P.Monceau),
Orsay (C.Brun and Z.Z.Wang),
Moscow (F.Nad, Yu.Latyshev)
Ljubljana (D.Mihailovic)
Singlet ground state gapful systems: SuperConductors SCs and Charge Density Waves CDWs.

Standard BCS-Bogolubov view:
Spectra: \[ E(k) = \pm (\Delta^2 + (v_f k)^2)^{1/2} \]
States = linear combinations of:
electrons and holes at \( \pm p \) for SC
electrons at \( -p \) and \( p + 2p_f \) for CDW

Figures: pair-breaking gaps from tunneling experiments.

Is it always true?
Proved “yes” for typical SCs.
Questionable for strong coupling: High-\( T_c \), real space pairs, cold atoms, bi-polarons.
Certainly incomplete for CDWs as proved by many modern experiments.
Certainly inconsistent for 1D and even quasi 1D systems as proved theoretically.

Guilty and Most Wanted: solitons and their arrays.
Incommensurate Charge Density Wave – ICDW \sim A \cos(2K_F x + \phi) ; A \sim \Delta

Order Parameter \( O_{\text{cdw}} = A \exp[i\phi] \)

Upper defect:
Vortex with a soliton in its core

Lower defect:
Pair of vortices embracing 2 chains
= two solitons at neighboring chains
= co-localization of 2 (4) electrons
Visualization of the $2\pi$ soliton = pre-fabricated electrons’ pair

*C. Brun and Z.Z. Wang* STM scan of NbSe$_3$

Left - experiment:
At the (red) front line the defected chain is displaced by half of the period.
Along the defected chain the whole period $\pm 2\pi$ is missed or gained –
a pair of electrons/holes is accommodated to the ground state.

Right - theory:
Plot of $2\pi$ soliton = 2e particle with corrections for the amplitude deformation.
Defected chain misses one period having $\frac{1}{2}$ of the period shift at the centrums
In green : reference frame = other chains .
Less apparent: the amplitude soliton = SPINON- the gap node carrying Spin=$\frac{1}{2}$ but
CHARGE=0
Experimental raw plot:
defected chain – in red,
neighboring chain – in green

Plot from another data showing the soliton

Modeling by the amplitude soliton, placing its center at the position of the CDW maxima.

Modeling by the amplitude soliton, placing its center at the position of the CDW node.

The CDW condensate is perceived here and their by nodes of amplitude – spinons - carrying selftrapped electrons at their mid-gap states
Dynamics of solitons in tunneling experiments on NbSe$_3$


**creation of the amplitude soliton at** $E_s = 2\Delta/\pi$

**All features scale with** $\Delta(T)$ **!**

- Peak $2\Delta$ for inter-gap creation of e-h pairs
- Absolute threshold at low $V_t \approx 0.2\Delta$
- And the oscillating fine structure - ground state reconstruction within the nano-junction – see the poster by Tianyou Yi

What tunnels at the subgap voltages? – all already seen by the STM!

1. Pair-breaking processes involving amplitude solitons at $E_s = 2\Delta/\pi$
2. Phase solitons with the energy $E_s \sim 3D$ ordering temperature $T_p$. 
**Puzzle and inspiration:**

Topologically nontrivial (amplitude) solitons were observed in 3D ordered phase, at $T < T_c$.

**Obstacle:** topological confinement:

Commutation between equivalent states on the chain results in loss of inter-chain energy $\sim$ total length: «confinement of kinks»

We need to activate other modes to cure the defect

**RESOLUTION – combined symmetry $U_1/Z_2$ of the order parameter $A \exp(i\varphi)$**

Amplitude soliton (kink) $A \leftrightarrow -A$, together with $\frac{1}{2}$-integer vortex of the phase $\varphi \rightarrow \varphi + \pi$, leaves invariant the order parameter

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Flux lines of $\frac{1}{2}$-vortices

Core: the kink – spin carrier

Kink – roton combination, example of the superconductor = CDW.


Splitting of orbital vortex at the presence of spins imbalance
Singlet Superconductivity – equivalence to ICDW

\[ O_{SC} \sim \psi_{+\uparrow} \psi_{-\downarrow} + \psi_{+\downarrow} \psi_{-\uparrow} \sim \exp \left[ i\chi \right] \cos \theta \quad H=...-g_1 \cos 2\theta \]

\[ \theta \rightarrow \theta + \pi \quad s=1/2 \]

\[ \uparrow \text{spin soliton} \uparrow \quad \chi \rightarrow \chi + \pi \quad \uparrow \text{wings of supercurrents} \uparrow \]

Quasi 1d view: spinon as a \( \pi \)-Josephson junction in the superconducting wire (applications: Yakovenko et al).

2D view: pair of \( \pi \)-vortices shares the common core bearing unpaired spin.

3D view: half-flux vortex stabilized by the confined spin.

Updown view: nucleus of melted FFLO phase in spin-polarized SC.
Half filled band with repulsion.
SDW rout to the doped Mott-Hubbard insulator.

\[ H_{1D} \sim (\partial \phi)^2 - U \cos(2\phi) + (\partial \theta)^2 \]

U - Umklapp amplitude
(Dzyaloshinskii & Larkin; Luther & Emery).

\( \phi \) - chiral phase of charge displacements
\( \theta \) - chiral phase of spin rotations.

Degeneracy of the ground state:
\[ \phi \rightarrow \phi + \pi = \text{translation by one site} \]

Staggered magnetization \( \equiv \text{AFM}=\text{SDW order parameter:} \)

\[ O_{SDW} \sim \cos(\phi) \exp\{\pm i(\mathbf{Q}x + \theta)\} , \text{amplitude } A = \cos(\phi) \text{ changes the sign} \]

To survive in \( D>1 \): The \( \pi \) soliton in \( \phi \): \( \cos \phi \rightarrow - \cos \phi \)
enforces a \( \pi \) rotation in \( \theta \) to preserve \( O_{SDW} \)

Propagating hole as an amplitude soliton.
Its motion permutes AFM sublattices \( \uparrow, \downarrow \)
creating a string of the reversed order parameter: staggered magnetization.
It blocks the direct propagation unless the 180 rotation is added.

Nagaev et al, Brinkman and Rice
Inverse rout: from stripes to solitons

$1D \rightarrow quasi\ 1D \rightarrow 2D,3D$ route to doping of AFM insulator. Aggregation of holes (extracted electrons) into stripes.

Left: scheme derived from neutron scattering experiments. Right: direct visualization via electron diffraction microscope.

Equivalence for spin-gap cases:
Fulde-Ferell-Larkin-Ovchinnikov FFLO phase in superconductors
Solitonic lattices in CDWs above the magnetic breakdown
Solitonic lattices in spin-Peierls GeCuO in HMF - Grenoble
Kink-roton complexes as nucleuses of melted lattices:
FFLO phase for superconductors or strips for doped AFMs.

Defect is embedded into the regular stripe structure (black lines).
+/- are the alternating signs of the order parameter amplitude.
Termination points of a finite segment L (red color) of the zero line must be encircled by semi-vortices of the $\pi$ rotation (blue circles) to resolve the signs conflict.
The minimal segment would correspond to the spin carrying kink.

Vortices cost $\sim E_{\text{phase}} \log L$ is less than the gain $\sim -\Delta L$
for the string formation at long $L$. Can we shrink to the atomic scale?
For smallest $L$~"unit cell", it is still valid in quasi 1D: $E_{\text{phase}} \sim T_c < \Delta$
For isotropic SCs, $E_{\text{phase}} \sim E_f$ – strong coupling is necessary.
(TMTCF)$_2$X, 1980 – Bechgaard, Jerome

SC- superconductivity  
AF- AFM = SDW  
SP- Spin-Peierls  
LL- Luttinger liquid  
MI- Mott insulator

Red line $T_{CO} – 2000$’s revolution:  
Ferroelectricity (Monceau, Nad, SB, et al)  
= Charge Ordering (Brown et al)

Views and interpretations:  
FerroElectric Mott-Hubbard state, 
mixed site/bond $4K_F$ CDW, non- 
symmetrically pinned Wigner crystal, 
charge ordering = disproportionation

Facility to see Solitons: 
purely 1D regime - 
$T_{CO} \approx 150K$ is 10 times 
above 3D electronic transitions.
Spinless charge carriers, holons:

Conductance $G$ (normalized to RT, Ahrenius plot $\log G$ versus $1/T$).

Clearlest example for conduction by charged spinless solitons - holons.

Conrarily to normal semiconductors, there is no gap in spin susceptibility $\chi$.

Gaps for thermal activation $\Delta$ range within 500-2000K.
1D Mott state = $4K_F$ CDW= commensurate Wigner crystal
Spin degrees of freedom are gapless and split-off.
Charge degrees of freedom: phase $\varphi=\varphi(x,t)$

$2K_F$ CDW/SDW $\sim\cos(\varphi+\pi x/a)$; $4K_F$ CDW $\sim\cos(2\varphi+\pi x/a)$

$$H = \left(\frac{\hbar}{4\pi\gamma}\right) \left[ v \left( \partial_x \varphi \right)^2 + \left( \partial_t \varphi \right)^2 \right] / v - U \cos(2\varphi-2\alpha)$$

Phase centre shift $\alpha$ - sign of the ferroelectricity
$U$ - Umklapp scattering amplitude, leading to the Mott state
$\gamma = K_\rho$ - major monitoring parameter
Ground state energy $H_U = -U \cos(2\phi - 2\alpha)$ is doubly degenerate between $\phi = \alpha$ and $\phi = \alpha + \pi$.
It allows for phase $\pi$ solitons, i.e. holons with the charge $e$.

$\phi = 0$

$\phi = \pi$

Purely on-chain solitons, exist as conducting quasiparticles both above and below the $T_{FE}$.

Spontaneous $\alpha$ itself can change sign between different FE domains. Then electronic system must also adjust its ground state from $\alpha$ to $-\alpha$.

Hence the phase soliton: increment $\delta \phi = -2\alpha$, 

*non integer* charge $q = -2\alpha/\pi$ per chain.

$\phi = -\alpha$

$\phi = \alpha$

alpha- solitons are walls between domains of opposite FE polarizations

They are on-chain conducting particles only above $T_{FE}$. Below $T_{FE}$ they aggregate into macroscopic walls. They do not conduct any more, but determine the FE depolarization dynamics.
Very high dc conductivity, but its Drude tail takes only 10% of the sum rule; The rest goes to the gap structure expected and seen in the Mott insulator case.

Optical absorption at the Mott gap coexisting with the Drude tail: A resemblance to normal pockets in under-doped cuprates?
Effects of subsequent transitions.

Combined solitons. Spin-Charge reconfinement.

Another present from the Nature: tetramerization in \((\text{TMTTF})_2\text{ReO}_4\) at \(T_{\text{AO}}<T_0\)

Spin-charge reconfinement below \(T_{\text{AO}}\) of tetramerisation. Enhanced gap \(\Delta\) comes from topologically coupled \(\pi\)-solitons in both sectors of the charge and the spin. The last is weakly localized.

What does it mean?

Spin degrees of freedom enter the game:

\[ \Psi_{\pm\sigma} \sim \exp[\pm i(\varphi + \sigma \theta / 2)] \]

\(\theta\) - spin phase, \(\theta'\)/ \(\pi\) = smooth spin density
Further symmetry lifting of lattice tetramerization or of spin-Peierls order mixes charge and spin: additional energy

\[ V\cos(\phi-\beta)\cos\theta \] - on top of \[ \sim U\cos(2\phi-2\alpha) \]

\( \phi \) and \( \theta \) -- chiral phases counting the charge and the spin

\( \phi' / \pi \) and \( \theta' / \pi \) = smooth charge and spin densities

\( \cos\theta \) sign instructs the CDW to make spin singlets over sorter bonds

Major effects of the small \( V \) - term :

Opens spin gap \( 2\Delta_\sigma \):

- triplet pair of \( \delta\theta=\pi \) solitons at \( \phi=\text{cnst} \)
- Prohibits \( \delta\phi = \pi \) solitons –
  now bound in pairs by spin strings
- Allows for combined spin-charge
  topologically bound solitons:

\[ \{\delta\phi = \pi, \delta\theta= \pi\} \] – leaves the \( V \) term invariant

Quantum numbers of the compound particle --
charge \( e \), spin \( 1/2 \) but differently localized:

charge \( e \), \( \delta\phi = \pi \) sharply within \( \hbar v_F/\Delta_p \)
spin \( 1/2 \), \( \delta\theta = \pi \) loosely within \( \hbar v_F/\Delta_\sigma \)
• Existence of solitons is proved experimentally in single- or bi-electronic processes of CDWs in several quasi 1D materials.
• They feature self-trapping of electrons into mid-gap states and separation of spin and charge into spinons and holons, sometimes with their reconfinement at essentially different scales.
• Topologically unstable configurations are of particular importance allowing for direct transformation of electrons into solitons.
• Continuously broken symmetries allow for solitons to enter D>1 world of long range ordered states: SC, ICDW, SDW.
• Solitons take forms of amplitude kinks, topologically bound to semi-vortices of gapless modes – half integer rotons.
• These combined particles substitute for electrons certainly in quasi-1D systems – valid for both charge- and spin- gaped cases
• The description is extrapolatable to strongly correlated isotropic cases. Here it meets the picture of fragmented stripe phases.