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Topological Excitations of Correlated Electronic States

One dimensional systems in the higher D world. Which of their wonders are preserved? Which new ones will appear? What knowledge will they bring?

Solitons in 2000's, WHY?

New conducting polymers,

- New events in organic conductors,
- New accesses to Incommensurate CDWs,

New approach to strongly correlated systems as semiconductors.

Elementary excitations in electronic systems with spontaneous symmetry breaking: Superconductors, Antiferromagnetic semiconductors or Mott Insulator, Spin/ Charge Density Waves (commensurate or not)

Secure starting level: one- dimensional systems. Solitons in the ground state and as elementary excitations. Conversion of electrons to various solitons; Separated or even anomalous charge, spin, currents.

Quasi one- dimensional route:

Confinement of solitons and dimensional crossover. Spin-charge recombination due to 3D confinement. Solitons acquire tails.

Arbitrary systems:

- Solitons acquire feathers.
- Combined symmetry of spin-charge transformations,
- Topological constraints and coupling, Spin- or Charge- roton like excitations with charge- or spin- kinks localized in the core.

- Combined symmetry breakings in polymeric and organic conductors *-- new routs to solitons.*
- **Charge Ordering** together with Bonds Dimerization:
- Peierls and Mott-Hubbard effects.
- Build-in extrinsic and spontaneous intrinsic effects.
- Nonequivalence of bonds and of sites.
- In any case (organic crystals or polymers) this combination lifts the inversion symmetry, hence the Ferroelctricity.

FERROELECTRIC MOTT-HUBBARD PHASE and CHARGE ORDERING in QUASI 1D ORGANIC CONDUCTORS.

- Collaboration: F. Nad
- Moscow and Grenoble
 - P. Monceau Grenoble and Saclay
 - J.M. Fabre & C. Carcel Montpellier.
- NMR route: S. Broun et al, UCLA
- *Event*: resolution for a longest (since 1985) story of misinterpretations: lost high T phase transitions.
- A challenge to the High-Tc world:
- Thought-to-be crossover lines may be true phase boundaries.



(TMTCF)₂X, 1980-2002 In black and white: SC- superconductivity AF-AFM = SDW**SP-** Spin-Peierls LL-Luttinger liquid **MI-** Mott insulator Red line - 2000 revolution: = Ferroelectricity = Charge disproportionation

Resolving the mystery of structureless transitions: Coulon et all, 1985 Gigantic anomaly in permitivity of $\varepsilon'(T)$ (Nad et al, Grenoble-Moscow) Charge Orderin seen by NMR (Brown - UCLA, Fujiyama -IMS).

Views and interpretations: FerroElectric version of Mott-Hubbard state, mixed site/bond 4K_F CDW, nonsimmetrically pinned Wigner crystal Facility to see Solitons: Purely 1D regime for electrons - $T_{FE} \approx 150$ is 10 times above 3D electronic transitions.



Why solitons, and as many as 4 types?

 $G \sim \exp(-\Delta/T)$

Solitons as spinless charge carriers:

- Conductance G normalized to RT, Ahrenius plot LogG(1/T).
- Gaps for thermal activation Δ range within 500-2000K.
- Clearlest example for conduction by
- charged spinless solitons holons.
- Conrarily to normal semiconductors no gap in spin susceptibility:
- Pauli-like χ =cnst as in the metallic high T phase.

COMBINED MOTT - HUBBARD STATE

 $\mathsf{H} \sim (\hbar/4\pi\gamma) \, [\mathsf{v}_{\rho} \ (\partial_{\mathsf{x}} \varphi \)^2 + (\partial_{\mathsf{t}} \varphi \)^2 / \mathsf{v}_{\rho} \] + \mathsf{H}_{\mathsf{U}}$

Chiral phase $\varphi = \varphi(x,t)$ for electrons near +/-K_F U: amplitude of the Umklapp scattering

2 types of dimerization \Rightarrow

2 interfering sources for two-fold commensurability

 \Rightarrow 2 contributions to the Umklapp interaction.

Site dimerization. : $H_U^s = -U_s \cos 2\varphi$ (spontaneous) Bond dimerization : $H_U^b = -U_b \sin 2\varphi$ (build-in) At presence of both site and bond types $H_U = -U_s \cos 2\varphi - U_b \sin 2\varphi = -U \cos (2\varphi - 2\alpha)$ $U = (U_b^{2} + U_s^{2})^{1/2}$, tan $2\alpha = U_s / U_s$ $U_s \neq 0 \Rightarrow \alpha \neq 0 \Rightarrow$ phase $\varphi =$ "mean displacement of all electrons" shifts from $\varphi = 0$ to $\varphi = \alpha$, hence the gigantic FE polarization.

From a single stack to a crystal: Macroscopic FerroElectric ground state if the same α is chosen for all stacks, Anti-FE state if the sign of α alternates as for (TMTTF)₂SCN.

For a given U_s the ground state is still doubly degenerate between $\varphi = \alpha$ and $\varphi = \alpha + \pi$. H_U = -Ucos (2 φ -2 α) It allows for phase π solitons, i.e. holons with the charge *e*.



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

Spontaneous U_s itself can change sign between different FE domains. Then the electronic system must also adjust its ground state from α to $-\alpha$. Hence the domain boundary $U_s \leftrightarrow -U_s$ requires for the phase soliton of the increment $\delta = -2\alpha$ which will concentrate the *non integer* charge $q=-2\alpha/\pi$ per chain.

$$\varphi = -$$
 Alpha- a domains

Alpha- solitons are the walls between domains of opposite FE polarizations.

They are on-chain conducting particles only above T_{FE} . Below T_{FE} they aggregate into macriscopic walls. They do not conduct any more, but determine the FE depolarization dynamics. Effects of subsequent transitions.

Combined solitons. Spin-Charge reconfinement.

Another present from the Nature: tetramerization in $(TMTTF)_2 ReO_4$ at $T_{AO} < T_0$



Spin-charge reconfinement below T_{AO} of tetramerisation. Enhanced gap Δ comes from topologically coupled π - solitons in both sectors of the charge and the spin. The last is weakly localized. What does it mean ? $\Psi_{\pm\sigma} \sim \exp[\pm i(\varphi + \sigma \theta/2)]$

Charge φ and spin θ phases as modulation of Fermi momenta. θ -- chiral phase of the spin spin σ =+/-1, θ'/π = smooth spin density

Former translations $x \rightarrow x+2$ are weakly prohibited. Allowed ones are $x \rightarrow x+4$ hence only $\varphi \rightarrow \varphi +2\pi$ at first sight.

Invariant Hamiltonian: H_{U} = -Ucos (2φ-2α) - Vcos (φ-β)cos θ V~ Δ_{σ}^{2} ≠0 at T<T_{ao} Δ_{σ} is the spin gap

Origin of V: singlet pair creation by external periodic potential.



 $2K_F$ scattering due to tetramerization

Further symmetry lifting after the tetramerization mixes charge and spin chanals: additional energy $V\cos(\varphi-\beta)\cos\theta$

 ϕ and θ -- chiral phases counting the charge and the spin ϕ $'\!/\,\pi$ and $\theta'\!/\,\pi$ = smooth charge and spin densities

Major effects of V-term :

- Opens spin gap $2\Delta_{\sigma}$: triplet pair of $\delta \theta = \pi$ solitons at $\varphi = cnst$
- 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 $\frac{1}{2}$ but differently localized: charge **e**, $\delta \phi = \pi$ sharply within $\frac{\hbar v}{\Delta_{\rho}}$ spin $\frac{1}{2}$, $\delta \theta = \pi$ loosely within $\frac{\hbar v}{\Delta_{\sigma}}$





Solitons in Optics

ETH group

 $\sigma(\omega)$: Optical Conductivity

PSEOUDGAP REGION IN TMTSF SUBFAMILY. Plausible interpretations in terms of solitons=kinks:

optically active mode of the FE polarization or Drude peak. Kink at $\omega < \omega_{peak}$:

Collective phason mode = exciton = bound pair of kinks

 $ω_{\text{peak}}$ =2Δ - 2-particle gap: pair of kink

-- call for photoconductivity experiments.

Solitons in tunneling: Incommensurate CDWs.

Yurii Latyshev, P. Monceau, S.B., et all; *Moscow, Grenoble, Orsay, Sendai.* Direct observation of solitons in tunneling on **NbSe**₃ and **TaS**₃ Expected thresholds at 2 Δ for two electrons, followed through a pseudogap down to the edge for electron \rightarrow soliton transition at $2\Delta/\pi$. *Preliminary results:*

Yu.Latyshev, P.Monceau, A.Sinchenko, L.Bulaevskii, S.Brazovskii, T.Kawae, T.Yamashita, "Interlayer tunneling spectroscopy of the charge density wave state in NbSe3", in Proceedings of the International Workshop on Strongly Correlated Electrons in New Materials (SCENM02), Journal of Physics A: **36**, (2003) 9323.

Details to be published.





CONTINUOUS SYMMETRIES

Solitons are stable energetically but not topologically.

Special significance: allowance for a direct transformation of one electron into one soliton.

- (Only 2→2 were allowed for kinks in discrete symmetries) Incommensurate CDWs = chiral Gross-Neveu model
- Order Parameter ~A(x)COS[Qx+φ]
- $\Delta = A \exp[i\varphi]$; A amplitude , φ phase
- Ground State with an odd number of particles:
- In 1D Amplitude Soliton AS $\Delta(x=-\infty) \Leftrightarrow \Delta(x=\infty)$
- via $A \Leftrightarrow -A$ at arbitrary φ =cnst.
- Spin $\frac{1}{2}$ and Charge **0**



Oscillating electronic density, Overlap soliton A(x), Midgap state =spin shape



Soliton trajectories in the complex plane of the order parameter. Red line: stable amplitude soliton. Blue line: intermediate chordus soliton within chiral angle θ (black radial lines). The value θ =100° is chosen which corresponds to the optimal configuration for the interchain tunnelling.



Selftrapping branches $V_n(\theta)$ for chordus solitons for fillings n = 1 (red line) and n=2 (green line), the energy $E_0(\theta)$ (blue line) of localized split-off state as functions of the chiral angle θ . Phase tails of the amplitude soliton AS:

Prohibited in **D>1** (including **1+1**) environment (confinement !) Allowed in **D>1** if acquires phase tails with the total increment $\delta \varphi = \pi \{A \rightarrow -A, \varphi \rightarrow \varphi + \pi\}$:

selfmapping of the order parameter $\Delta = A \exp[i\varphi]$ Result: allowed particle with the AS core carrying the spin 1/2 plus the phase twisting wings carrying the charges e/2



Injecting a bare electron at a time **t=0**, AS core develops fast but the phase tails propagate (arrows) with the phase sound velocity **u**.

Tails contribute to the action $\sim u^{-1}ln[t]$. Hence the probability l(E) to create the AS near its threshold energy $E_{AS}=2/\pi\Delta$ is $l\sim(E-E_{AS})^{-1/u}$ This is the pseudogap between Δ and E_{AS} *S.Matveenko and S.B.*

Can the solitons cross the boarder to the higher D world ? Are they allowed to bring their anomalies like spin-charge separation or midgap states? Password : confinement.

As topological objects connecting degenerate vacuums, solitons acquire an infinite energy unless they reduce or compensate their topological charges.

Various scenarios :

- Compensation by the gapless mode S.B. 1980, 2000
- Aggregation into domain walls versus their melting by thermal deconfinement or long rage Coulomb forces S.B. & T.Bohr 1983, S. Teber 2001
- Coupling to structural defects in polymers.
- Binding to kink-antikink pairs, origin of bipolarons.
 S.B. & N.Kirova, 1981-90's
- Today's speciality : Topological binding to gapless degrees of freedom

Fatal effect upon kinks: lifting of degeneracy, hence confinement. Trivial but spectacular example: global lifting of symmetry.



Nature present: cis-isomer of (CH)_x Build-in slight inequivalence of bonds.

Confinement of kinks pairs into

2e charged (bipolaron) or neutral (exciton) formation.

Symmetry determined picture of optical differences for trans- and cis (CH)x.

Photoconductivity versus photoluminescence,

new optical features due to hybridization of midgap states.

S. B. and N. Kirova, 1981: Interpretation of experiments and «accidental» exact solution for the model with confinement.

FINITE TEMPERATURE, ENSEMBLES OF SOLITONS, PHASE TRANSITIONS OF CONFINEMENT AND AGGREGATION. DISCRETE SYMMETRY only.

Fatal effect upon kinks: lifting of degeneracy, hence confinement. Nontrivial but still spectacular:

local lifting in the state with long range order.

Interchain coupling of the order parameter. Two competing effects:

$$H_I = -\sum_{\langle \alpha, \beta \rangle} \int dx V_\perp \Delta_\alpha(x) \Delta_\beta(x)$$

Binding of kinks into pairs at $T < T_c$;

Aggregation into macroscopic domain walls at $T < T_0 < T_c$.



Solution for a statistical model T.Bohr and S.B. 1983, S.Teber et al 2000's

Quantum models based on bosonisation.

MIXED DISCRETE AND CONTENEOUS SYMMETRIES.SPIN-GAP cases.-↑H_{1D}~(∂θ)² -Vcos(2θ)} +(∂φ)²-↓V - from the backward exchange scatteringIIn 1D : Spinon as a soliton θ→ θ+π hence s=1/2;+↓Gapless charge sound in φ.CDW order parameter ~ ψ[†]_{+↑} ψ_{-↑} + ψ[†]_{+↓} ψ_{-↓} ~ exp [iφ] cosθ

At higher D : allowed mixed configuration $\theta \rightarrow \theta + \pi$, s=1/2 $\phi \rightarrow \phi + \pi$, e=1^fspin soliton ^^fcharged wings^

Spinon as a soliton + semi dislocation loop = π - vortex of $\phi \equiv$ confined spin + semi dislocation loop





Quasi 1d view : spinon as a π- Josephson junction in the superconducting wire (*applications: Yakovenko et al*).
 2D view : pair of π- vortices shares the common core bearing unpaired spin.

3D view : half-flux vortex stabilized by the confined spin. Best 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} ~($\partial \phi$)² -Ucos(2 ϕ)} +($\partial \theta$)²

U - Umklapp amplitude
(*Dzyaloshinskii & Larkin ; Luther & Emery*).
φ - chiral phase of charge displacements
θ - chiral phase of spin rotations.
Degeneracy of the ground state:

 $\phi \rightarrow \phi + \pi =$ translation by one site

Excitations in 1D :

holon as a π soliton in φ , spin sound in θ .

Higher D : A hole in the AFM environment.

Staggered magnetization = AFM=SDW order parameter:

- In a stretched frame of particles : $S \pm \sim \exp{\{\pm i(Qx + \theta)\}}$
- In the absolute frame of sites : $O_{SDW} \sim cos\phi \exp{\pm i(Qx+\theta)}$

To survive in D>1 : The π soliton in φ cos $\varphi \rightarrow$ - cos φ enforces a π rotation in θ 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: the staggered magnetization. It blocks the direct propagation. *Brinkman and Rice, Nagaev et al*



Adding the semi-vorticity to the string end heals the permutation thus allowing for propagation of the combined particle. Resulting Elementary Excitations:

half integer vortex ring of staggered magnetization = $\frac{1}{2}$ roton with the holon confined at its core.



Alternative view:

- Nucleus of the stripe phase or
- the minimal element of its melt.

- Physical variables :
- Electric charge -- Localized in the core;
- Delocalized AFM staggered and net ferro magnetizations.
- Well away from the core:

$$e^{i\theta} = \sqrt{\frac{x + i(y-1)}{\sqrt{x^2 + (y-1)^2}} \frac{x - i(y+1)}{\sqrt{x^2 + (y-1)^2}}}$$

$$S_{afm} \propto \frac{x}{x^2 + y^2} \qquad S_{fer} \propto \frac{(x^2 - y^2)}{(x^2 + y^2)^2}$$

E.g. to be tested by the NMR

Paradox:

the central chain, y=0: $\delta\theta=\pi \rightarrow s=1/2$ like an added electron of spin s=1/2, charge e=1. But integrally over cross section: $\int \delta \theta d^2 r_1 = 0 \implies \text{net spin} \quad \mathbf{s} = \mathbf{0}$ 3D quantum numbers are like for normal electron spin **s=1/2** (while in wings) charge **e=1** (while in the core). But integrally over a perpendicular cross-section: net AFM spin $S_{afm}=0$; integrally over any cross section: net magnetization **S**_{fer}=0

The LRO in D>1 reconfines the charge and the spin but only in a core. But integrally one of the two is transferred to the collective mode. Locally we restore single electronic quantum numbers but with different scales of localization. Integrally – still the spin without the charge. $1D \rightarrow quasi \ 1D \rightarrow 2D, 3D$ route to dopping of AFM insulator. Aggregation of holes (extracted electrons) into stripes. Left: scheme derived from neutron scattering experiments. Right: *direct visualization via electron diffraction microscope*.

<†₽	•	€↓Þ	(†)	(↓)	•	(†)
41D	() k	(†)	€↓₽	(†)		< LD
(†D	•	€ ↓)	(†)	€↓₽	•	(1)
4 1 B	0	(TP	4 4 0	<†>	\bullet	< L D
4 † B		4↓₽	€ ♠₽	4↓₽		(†)
41D	C 1	(†)	4↓₽	(†)		€↓₽
(†)	•	€ ↓ }	(+)	(↓)	•	(†)
4 L D	0	(1)	€↓₽	(↑)		(1)

J.Orenstein et al Science 288, 468 (2000)



S.Mori et al Nature 392, 473 (1998)

Equivalence for spin-gap cases:

Fulde-Ferell-Larkin-Ovchinnikov FFLO phase in superconductors Solitonic lattices in CDWs above the magnetic breakdown Kink-roton complexes as nucleuses of melted macro structures: FFLO phase for superconductors or strips for doped AFMs.



A defect embedded into the regular stripe structure (black lines). +/- are the alternating signs of the order parameter amplitude. Termination points of a finite segment (red color) of the zero line must be encircled by semi-vortices of the π rotation (blue circles) to resolve the signs conflict. The minimal segment corresponds to the spin carrying kink.

SUMMARY

- •Existence of solitons is proved experimentally in single- or bi-electronic processes of 1D regimes in quasi 1D materials.
- •They feature selftraping of electrons into midgap 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 int solitons.
- •Continuously broken symmetries allow for solitons to enter the D>1 world of LRO states: SC, ICDW, SDW.
- •They take forms of amplitude kinks topologically bound to semi-vortices of gapless modes.
- •Charge and spin can be viewed as reconfined or not depending on the type of measurement.
- •These combined particles substitute for electrons in all quasi-1D.
- •The picture is extrapolated to strongly correlated isotropic cases.

Supplementary sets of viewgraphs Page: <u>http://ipnweb.in2p3.fr/~lptms/membres/brazov/seminars.html</u>

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Brinkman and Rice Fukuyama and Tanaka Kirova and S.B. **Kusmartsev** Luther and Emery Matveenko Nagaev Shriman and Sigia Varoquaux Volovik Zaanen etc., etc.