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Topological Excitations of Correlated Electronic States: the rout from D=1 to higher dimensions

Expectations - Understanding of :

Spin-Charge separation and reconfinement

Forms of holons and spinons beyond 1D

Transfer of experimental information

Key words: solitons, instantons, complex topological defects

Solitons in 2000's, WHY?

New conducting polymers,

New events in organic conductors,

New accesses to Charge Density Waves,

New interests in strongly correlated systems as semiconductors

Elementary excitations in electronic systems with spontaneous symmetry breaking - The STRATEGY :

Symmetries: 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.

SOLITONS in Solid State Physics– WHERE, WHEN, WHY.

Solitons as classical excitations in 1D -- early 70's theories :

Magnetic chains, Charge Density Waves, Commensurability transition etc.

Schrieffer, Krumhansl, Rice, Bishop, McMillan, Dzyaloshinskii & S.B., …

Solitons in quantum electronic (*Sine-Gordon*) models --

mid 70's theories *Luther, Emery, Maki, et al; (in FT: Neveu et al, Coleman,…)*

Solitons and their stripes in 1D Quantum Semiconductors : *Gap opened by a spontaneous symmetry breaking due to electronic instabilities*.

Peierls–Frohlich-SSH models; Polyacethelene impact, -- around 1980

Pacific line: *Schrieffer, Su, Heeger, Maki, Takayama, Bishop, Campbell, ….,*

East-Euro line: S.B., Kirova, Matveenko, Dzyaloshinskii, Gorkov, …

A surprise from exact solutions and simulations:

well behaved *normal* electronic spectra in the ground state develop spin-charge *anomalies* for excited states –

via formation of amplitude and mixed solitons, mid-gap states.

Late 90's passage of solitons: pair breaking magnetic fields – CuGeO, BEDT.

Solitons in 2000's, WHY?

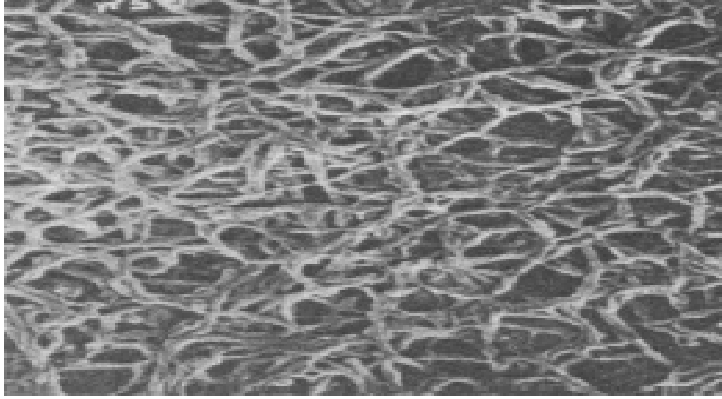
New events in organic conductors,

New accesses to Incommensurate CDWs,

New trends to use strongly correlated systems as semiconductors

(CERC-AIST, ISSP - Japan)

Heeger, MacDiarmid and Shirakawa
Nobel Prize in chemistry 2000
« for the discovery and development of electrically conducting polymers ».
Inside these noodles: *trans-(CH)$_x$* chains with one excess electron per site.

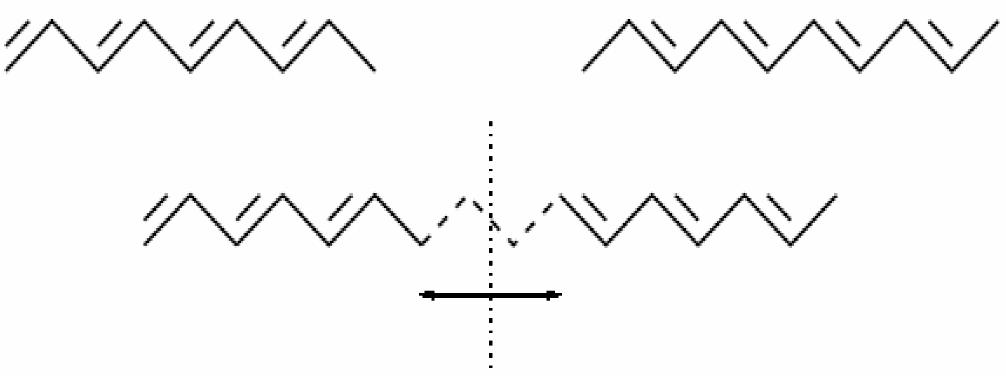


Chains should be metallic (gapless 1D electrons=fermions).
Instead, the interaction with atomic displacements=bosons develops their condensate=dimerization leading to the "spontaneous mass generation"=gap 2Δ for fermions.
Peierls effect, equivalence to Gross-Neveu model.

Ground state double degeneracy allows for topological solitons=kinks=
trajectories connecting equivalent vacuums (+/-1).

$$Tr\begin{vmatrix} -i\partial_x & \Delta^* \\ \Delta & i\partial_x \end{vmatrix} + K\overline{|\Delta|^2}$$

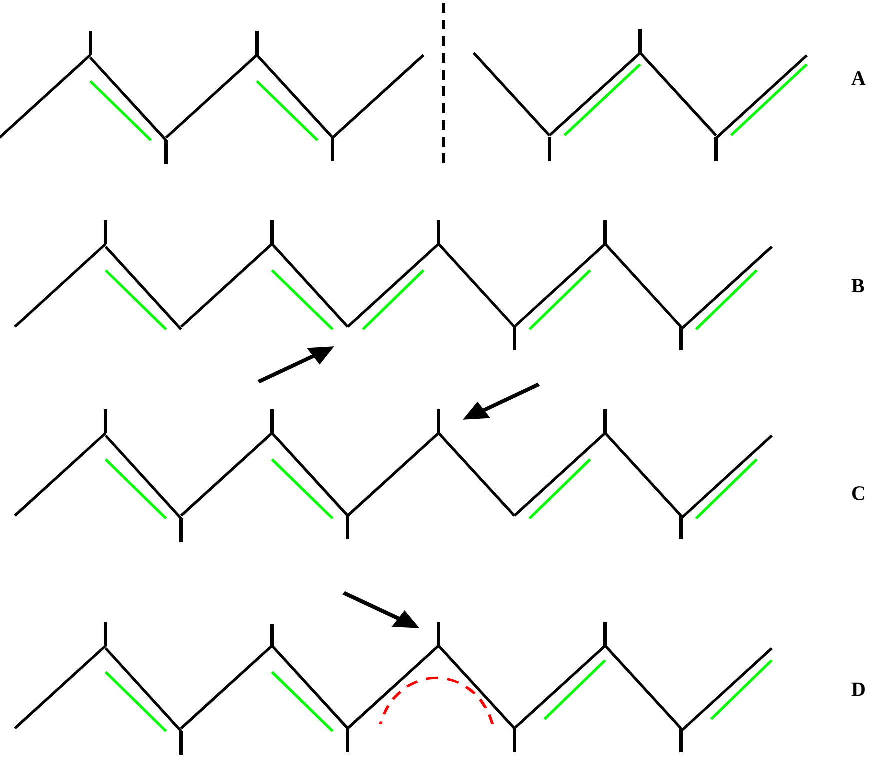
Phase of Δ is fixed, Z_2



Major properties of kinks:

1. Their energy < Δ: selftrapping of electrons into kinks (2→2)
2. They bear mid-gap states= zero fermionic mode
3. They carry either charge or spin

Topological defects on the trans-(CH)x chain

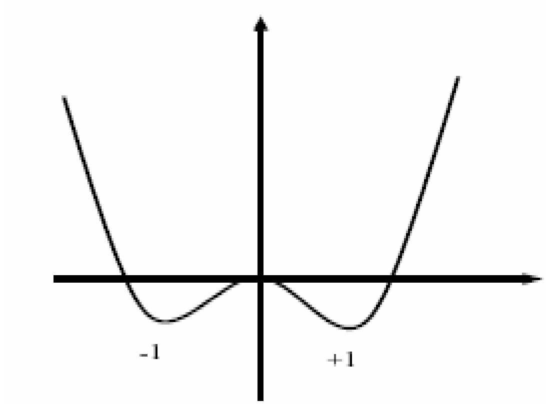


q=e, s=0

q=-e, s=0

q=0, s=1/2

Symmetry breaking - bond dimerization.
Two equivalent ground states.
Soliton= kink between them



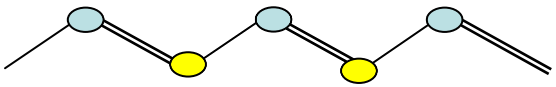
S.B., 1978; A.J. Heeger, R.J.Schrieffer, 1979; Takayama et al, 1980

SOILITONS WITH NONINTEGER VARIABLE CHARGES:

Orthogonal mixing of static and dynamic mass generations.

Realisation: modified polyacetylene $(CRCR')_x$ (K.Akagi, Tsukuba).

Theories for solitons with variable charges: S.B. & N.K. 1981, E.Mele and M.Rice



$$\Delta = \sqrt{\Delta_{ex}^{2} + \Delta_{in}^{2}}$$

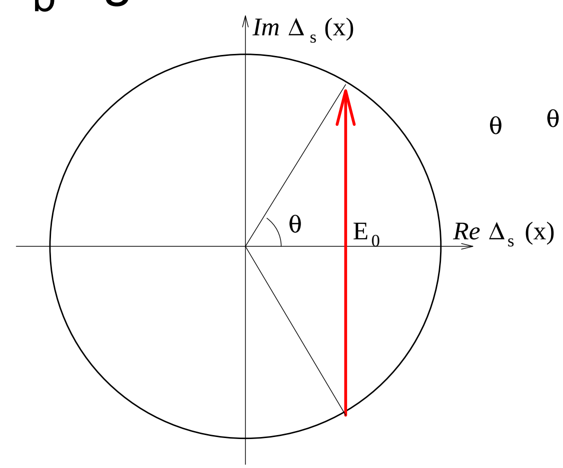
Joint effect of extrinsic Δ_{ex} and intrinsic Δ_{in} contributions to dimerization gap Δ.

Δ_{ex} comes from the build-in site dimerization – inequivalence of sites A and B.

Δ_{in} - from spontaneous dimerization of bonds $\Delta_{in}=\Delta_b$ - generic Peierls effect.

$$Tr\begin{vmatrix} -i\partial_x & \Delta_1 + i\Delta_2 \\ \Delta_1 - i\Delta_2 & i\partial_x \end{vmatrix} + K\overline{|\Delta_2|^2}$$

$$\Delta_1 = cnst, \quad \overline{\Delta_2} = \pm\sqrt{\Delta_0^2 - \Delta_1^2}$$

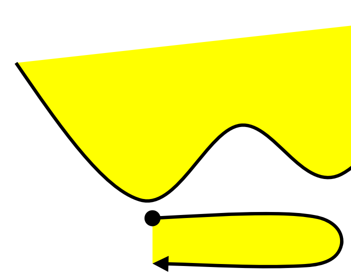


Nontrivial chiral angle 0<2θ<π of the soliton trajectory corresponds to the noninteger electric charge q= eθ/π

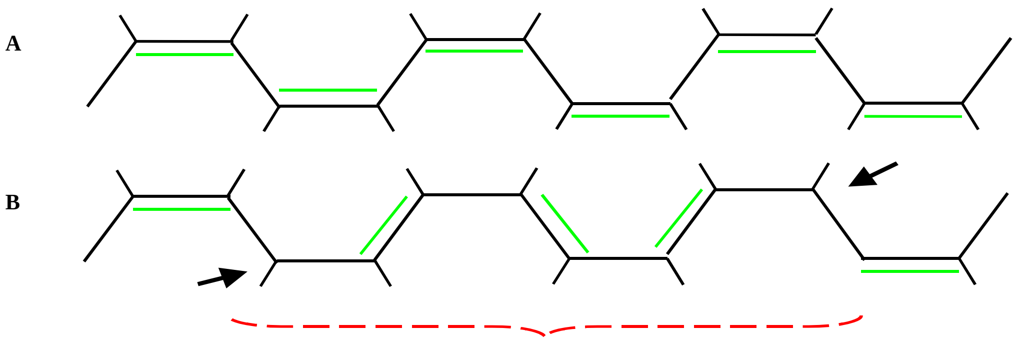
Fatal effect upon kinks: lifting of degeneracy, hence confinement.
Trivial but spectacular example: global lifting of symmetry.

Nature present -- cis-isomer of $(CH)_x$:
build-in slight inequivalence of bonds
hence lifting of ground state degeneracy,
hence confinement of solitons

Cis-$(CH)_x$:
Nonsymmetric dependence
of GS energy on dimerisation



Only a short excursion
= confined pair of kinks=
to the false GS is allowed



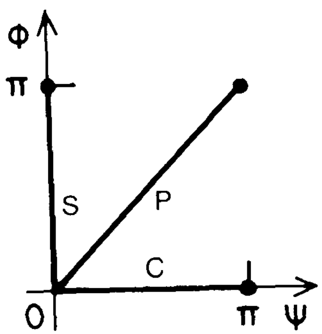
Confinement of kinks pairs into
2e charged (bipolaron) or neutral (exciton) compex.
Symmetry determined picture of optical differences for
trans- and cis- isomers *S. B. and N. Kirova, 1981*
Photoconductivity trans-$(CH)_x$ versus photoluminescence cis-$(CH)_x$
also new optical features due to hybridization of midgap states

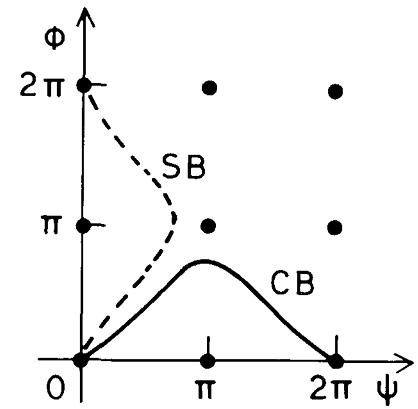
Confinement of different gapful degrees of freedom.
H. Fukuyama and H. Takayama 1985
DYNAMICAL PROPERTIES OF QUASI 1D CONDUCTORS

Dimerized Case (M = 2) - half-filled band:

$$\int dx\ [A_\rho(\nabla\psi)^2 + A_\sigma(\nabla\phi)^2 - B_\rho \cos 2\psi + B_\sigma \cos 2\phi +$$

$$+ K' u^2 - 2\tilde{g} u \cos\psi \cos\phi],$$





Classifications of solitons in the dimerized system correspond to the configuration in the ground state. Fundamental types of solitons are those denoted as C, S, and P;

C(Charge Soliton) Q = ±e, S = 0,
S(Spin Soliton) : Q = 0, S = ±1/2,
P(Polaron) Q=±e, S±l/2.

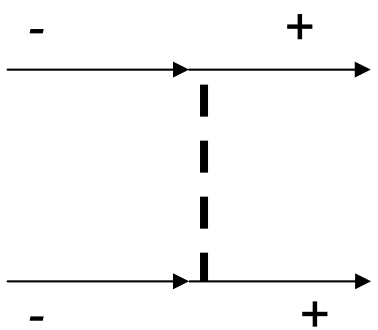
1D Mott-Hubburd state. 1 electron per site, i.e. the half filled band.

Spin degrees of freedom are split-off and gapless (free spin rotation phase θ).

Charge degrees of freedom can be gapful.

Chiral phase $\varphi=\varphi(x,t)$ for electrons near $+/-K_F$: $\Psi_{\pm} \sim \exp[\pm i\varphi/2]$

Origine: Umklapp scattering (Dzyaloshinskii & Larkin, Luther & Emery)



$U\exp[i2\varphi]$ *: amplitude of the Umklapp scattering of electrons* $(-K_F,-K_F) \rightarrow (+K_F,+K_F)$ is allowed here. Momentum deficit $4K_F$ is just compensated by the reciprocal lattice period. Continuous chiral symmetry lifting: arbitrary translations are forbidden on the lattice. Remnant symmetry: Allowed translations $x\rightarrow x+2$ hence $\varphi\rightarrow\varphi+\pi$ is preserved.

$$H\sim (\hbar/4\pi\gamma)\,[v_\rho\,(\partial_x\varphi)^2 + (\partial_t\varphi)^2/v_\rho] - U\cos(2\varphi)$$

Hamiltonian degeneracy $\varphi\rightarrow\varphi+\pi$ originates current carriers:

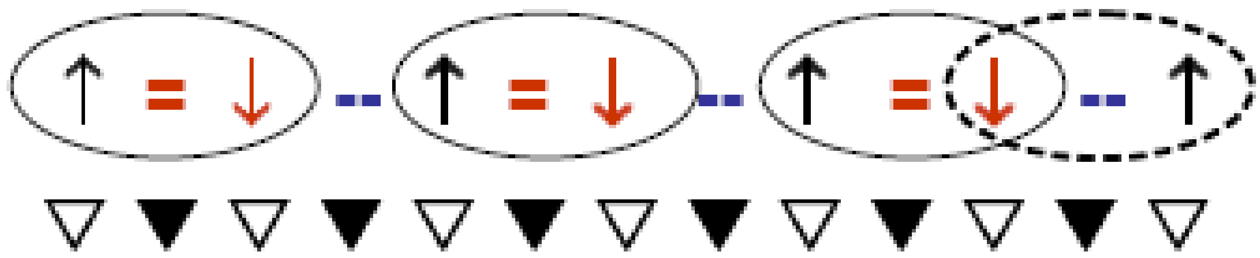
$\pm\pi$ solitons with charges $\pm e$, energy Δ

(= holon = $4K_F$ CDW discommensuration = Wigner crystal vacancy)

Stability conditions:

$\gamma<1$: U is not renormalized to zero if already present - common case

$\gamma<1/2$: U can be spontaneously generated - new circumstances



Schematic illustrations for effects of the tetramerization

Inequivalence of bonds **=** , **--** between good sites ▽ endorses ordering of spin singlets.

Also it prohibits translations by one ▽ ▼ ▽ distance which were explored by the $\delta\varphi\boldsymbol{=\pi}$ soliton.

But its combination with the defected unpaired spin ($\delta\boldsymbol{\theta=\pi}$ soliton which shifts the sequence of singlets) is still allowed as the selfmapping –

connction of equivalent ground states

Further symmetry lifting of tetramerization mixes charge and spin:
additional energy **$V\cos(\varphi-\beta)\cos\theta$** – on top of **$\sim V\cos(2\varphi)$**

φ and θ -- chiral phases counting the charge and the spin

φ'/π and θ'/π = smooth charge and spin densities

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

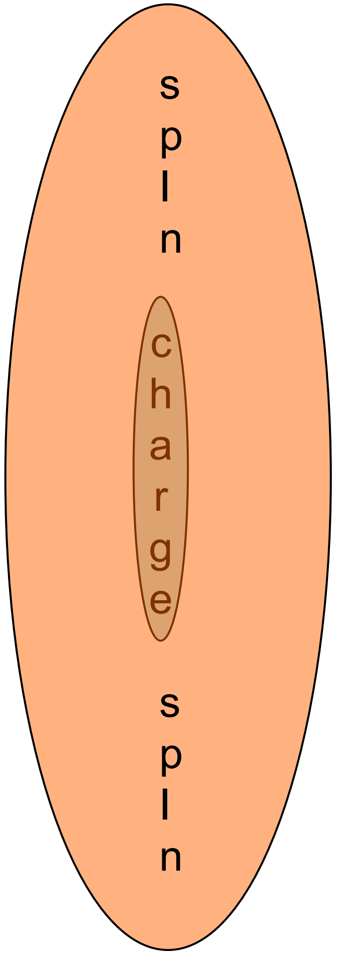
Major effects of V-term :

Opens spin gap **$2\Delta_\sigma$** :

triplet pair of $\delta\boldsymbol{\theta}\mathbf{=}\pi$ solitons at φ=*cnst*

- Prohibits $\delta\varphi\,\mathbf{=}\pi$ solitons –
  now bound in pairs by spin strings
- Allows for combined spin-charge
  topologically bound solitons:

$\{\delta\varphi=\pi+\delta\boldsymbol{\theta}=\pi\}$ – leaves the **V** term invariant



Quantum numbers of the compound particle --

charge **e** , spin ½ but differently localized:

charge **e** , $\delta\varphi\,\mathbf{=}\pi$ sharply within $\hbar v_F/\Delta_\rho$

spin **½** , $\delta\boldsymbol{\theta}\,\mathbf{=}\pi$ loosely within $\hbar v_F/\Delta_\sigma$

Contineous symmetries.

Solitons 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)*

Peierls-Fröhlich model for incommensurate CDWs

= chiral Gross-Neveu model in field theory

Order Parameter $O_{cdw} \sim A(x)\,\mathrm{COS}[Qx+\varphi]$

$$Tr\begin{vmatrix} -i\partial_x & \Delta^* \\ \Delta & i\partial_x \end{vmatrix} + K\overline{|\Delta|^2}$$

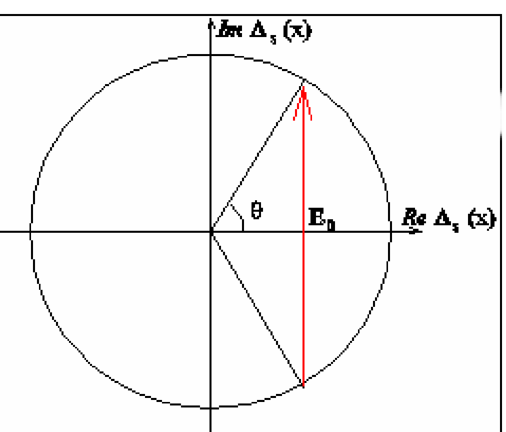
Δ= A exp[iφ]; A - amplitude , φ - phase

Ground State with an odd number of particles:

In 1D - *Amplitude Soliton* AS $\Delta(x=-\infty) \Leftrightarrow -\Delta(x=\infty)$

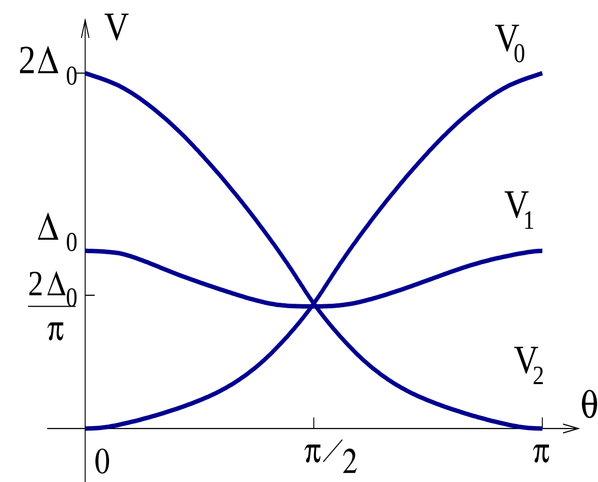
via A $\Leftrightarrow$-A at arbitrary φ=cnst.

Spin ½ and Charge 0 (*fractional variable charge at circumstances: S.B., Dzyaloshinskii, Kirova, Matveenko*)



Sequence of chordus solitons develops from bare θ=0 through AS 2θ=π to the full phase slip 2θ=2π.

Midgap state evolves from Δ_0 to $-\Delta_0$ providing spectral flow across the gap.



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's*
- 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

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.

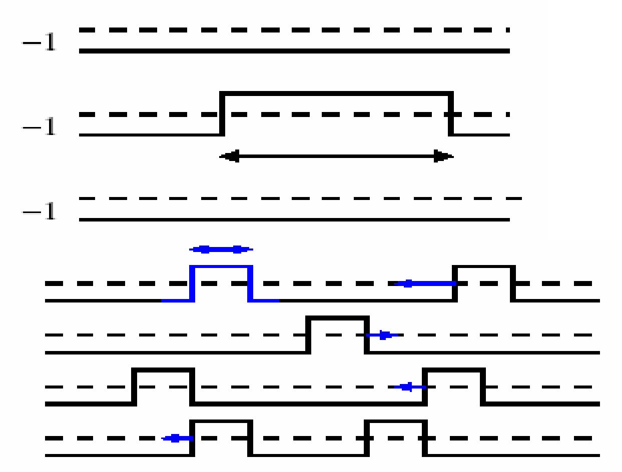
Interchain coupling of the order parameter.

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

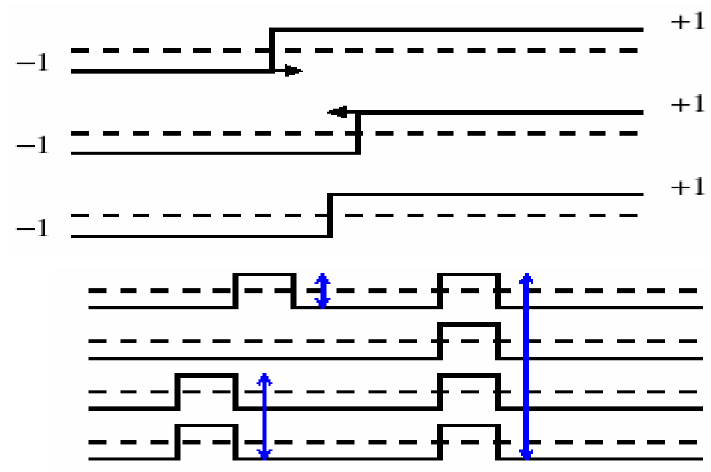
Two competing effects:

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

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



T > To



T < To

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

Why did we see the single solitons ? :

combination of a discrete and continuous symmetries

Solitons are stable energetically but not topologically

Recall a general theory: Mineev & Volovik, Toulouse, etc.

Special significance: allowance for a direct transformation of

one electron into one soliton.

(Only 2→2 *were allowed for kinks in discrete symmetries)*

Incommensurate CDW Order Parameter **~A(x)COS[Qx+φ]**

Δ= A exp[iφ] ; **A** - amplitude , φ - phase

Ground State with an odd number of particles:

In 1D - *Amplitude Soliton* AS **Δ(x=-∞) ⇔ - Δ(x=∞)**

via **A** ⇔**-A** at arbitrary φ=cnst

Favorable in energy in comparison with an electron, but:

Prohibited to be created dynamically in 1D

Prohibited to exist even stationary at D>1

RESOLUTION – Combined Symmetry :

Phase tails of the amplitude soliton AS:

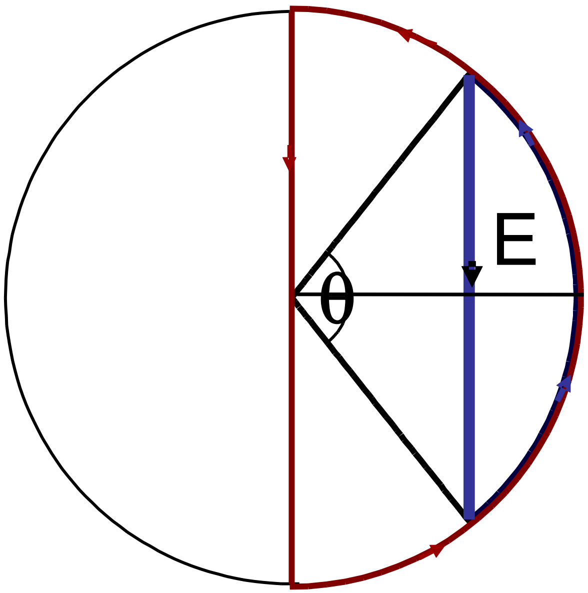
Prohibited in **D>1** (including **1+1**) environment (confinement !)

Allowed in **D>1** if acquires phase tails with the total increment

$\delta\varphi=\pi$ {A → -A, φ → φ + π} :

Self-mapping of the order parameter **Δ= A exp[iφ]**

Result: allowed particle with the AS core carrying the spin **1/2** plus the phase twisting wings carrying the charges **e/2**



Soliton trajectories in the complex plane of the order parameter Aexp(iϕ) .
Red vertical line: stable amplitude soliton.
Blue line: intermediate chordus soliton within chiral angle θ (black radial lines).
θ=100° is chosen - optimal configuration for interchain tunnelling *Matveenko & SB*
Arc lines: adaptational phase tails

π-rotation accumulated in the phase tails
is generalized as an effect of :
pair of **half- integer** vortices (D=2) or of such a vortex ring (D=3)

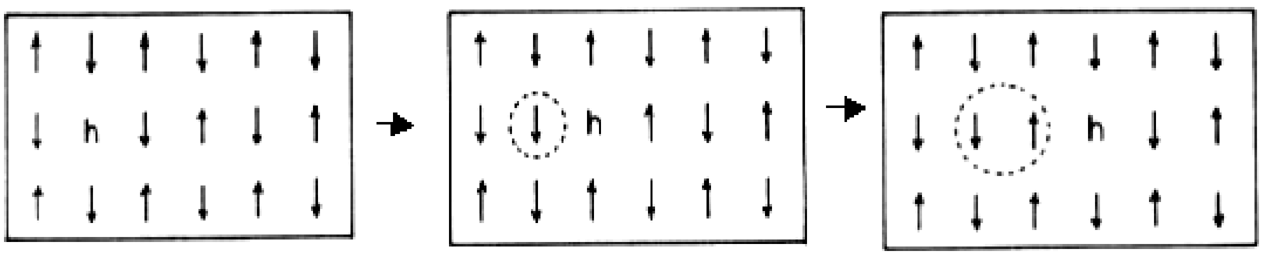
Propagating hole as an amplitude soliton.

Its motion permutes AFM sublattices ↑,↓

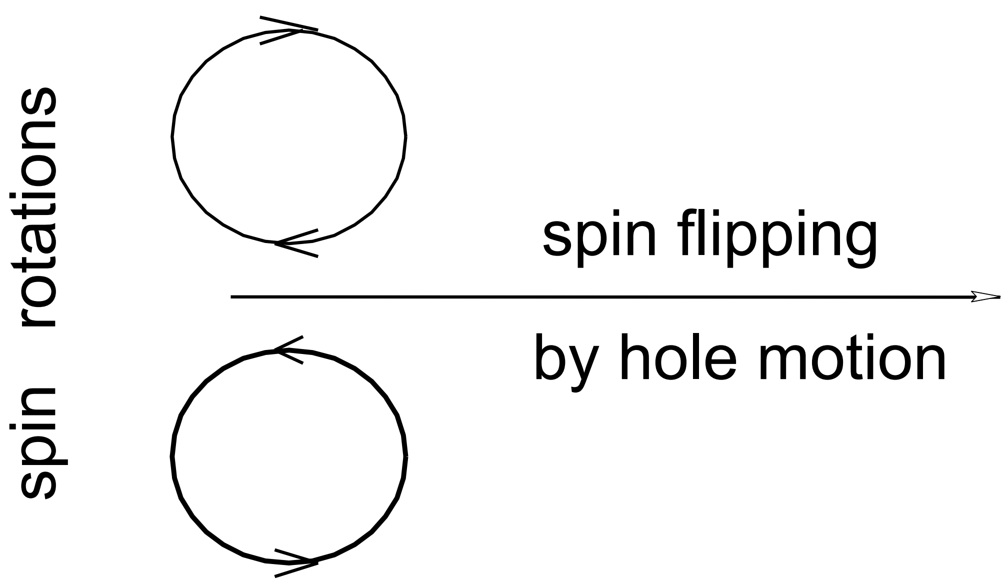
creating a string of the reversed order parameter:

staggered magnetization.   It blocks the direct propagation.

Nagaev et al , Brinkman and Rice



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



Half filled band with repulsion.
SDW rout to the doped Mott-Hubbard insulator.

$$H_{1D} \sim (\partial\varphi)^2 - U\cos(2\varphi)\} + (\partial\theta)^2$$

U - Umklapp amplitude

(*Dzyaloshinskii & Larkin ; Luther & Emery*).

φ - chiral phase of charge displacements

θ - chiral phase of spin rotations.

Degeneracy of the ground state:

$\varphi \to \varphi+\pi$ =   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 $\equiv$ AFM=SDW order parameter:

$$\mathbf{O_{SDW} \sim \cos\varphi \exp\{\pm i(Qx+\theta)}$$

To survive in D>1 :

The π soliton in φ cos $\varphi \to$ - cos φ

enforces a π rotation in θ to preserve O_{SDW}

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

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

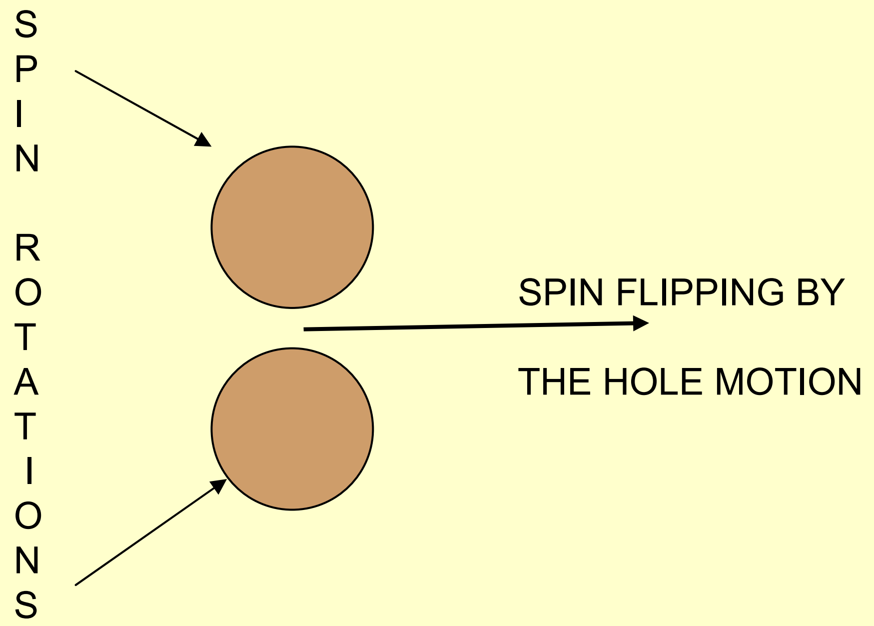
$$S_{\mathrm{afm}} \propto \frac{\mathrm{x}}{\mathrm{x}^2+\mathrm{y}^2} \qquad S_{fer} \propto \frac{(\mathrm{x}^2 - \mathrm{y}^2)}{(\mathrm{x}^2 + \mathrm{y}^2)^2}$$

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:
  $\int\delta\theta d^2r_\perp=0 \Rightarrow$ net spin s=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 the any cross section:
  net magnetization $S_{fer}=0$
- The D>1 reconfines the charge and the spin but only in a core. 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.

Resulting Elementary Excitations:

half integer vortex ring of staggered magnetization = ½ roton with the holon confined at its core.



Alternative view:

Nucleus of the stripe phase or

the minimal element of its melt.

MIXED DISCRETE AND CONTENEOUS SYMMETRIES.

SPIN-GAP cases: Incommensurate CDW or Superconductor

$H_{1D} \sim (\partial\theta)^2$ **-Vcos(2θ)}** $+(\partial\varphi)^2$

V - from the backward exchange scattering of electrons

In **1D** : Spinon as a soliton $\theta \rightarrow \theta+\pi$ hence **s=1/2**

+ Gapless charge sound in φ.

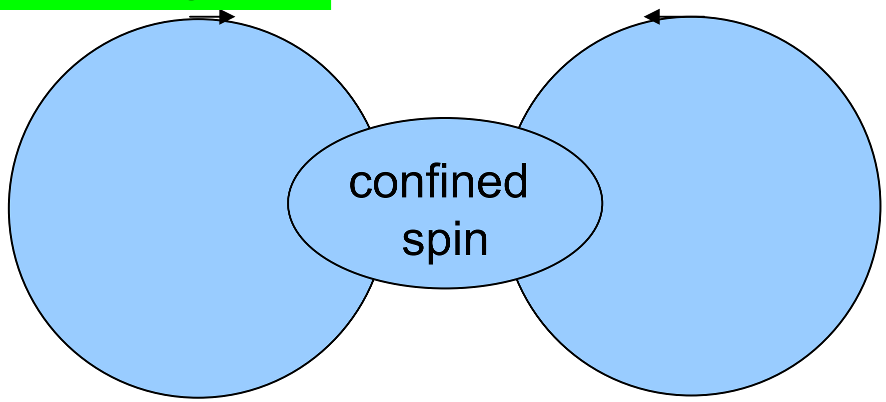
CDW order parameter $\sim \psi^{\dagger}_{+\uparrow}\psi_{-\uparrow} + \psi^{\dagger}_{+\downarrow}\psi_{-\downarrow} \sim \exp[i\varphi]\cos\theta$

At higher D : allowed mixed configuration

$\theta \rightarrow \theta+\pi$, **s=1/2** $\varphi \rightarrow \varphi+\pi$, **e=1**

↑spin soliton ↑ ↑charged wings↑

Spinon as a soliton + semi-integer dislocation loop = π - vortex of φ ≡ confined spin + semi dislocation loop

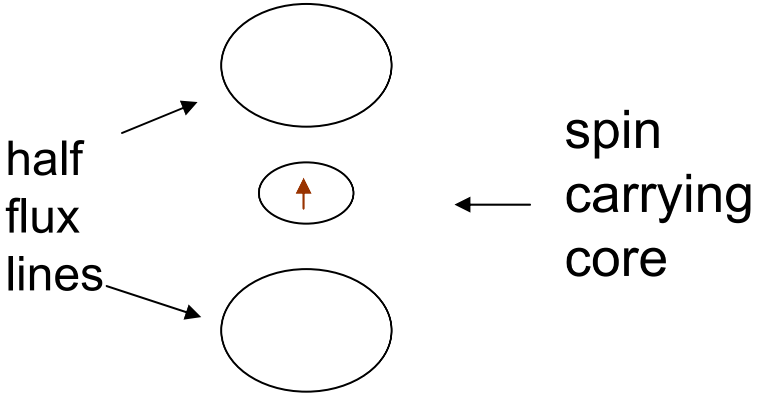


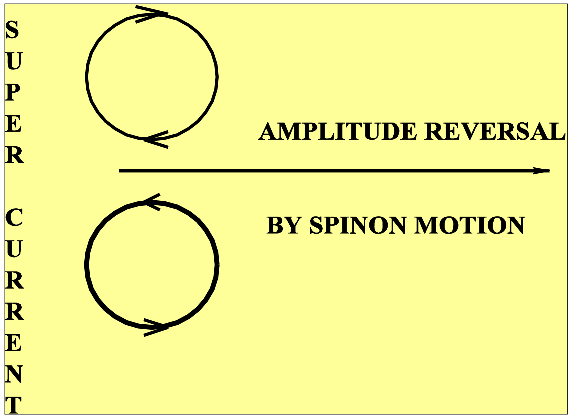
Singlet Superconductivity: D=1 → D>1

$$\eta_{SC} \sim \psi_{+\uparrow}\,\psi_{-\downarrow} + \psi_{+\downarrow}\,\psi_{-\uparrow} \sim \exp[i\chi]\cos\theta$$

$\theta \to \theta+\pi$ s=1/2 $\qquad\qquad$ $\chi \to \chi+\pi$

↑spin soliton ↑ $\qquad\qquad$ ↑wings of supercurents↑





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.

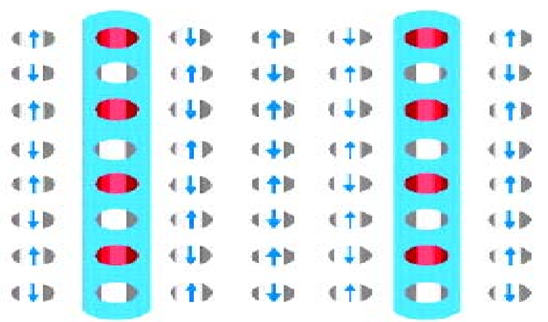
3D view : half-flux vortex stabilized by the confined spin.

Best view: nucleus of melted FFLO phase in spin-polarized SC

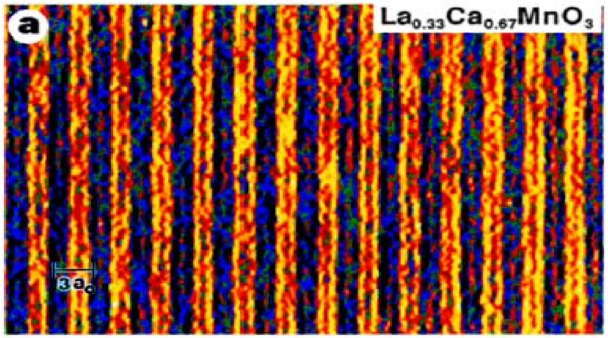
Inverse rout: from stripes to solitons

1D → quasi 1D → 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.*



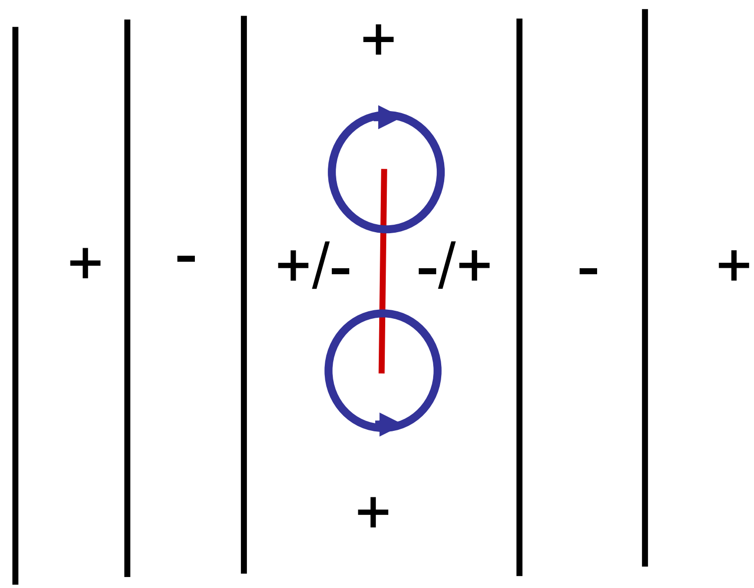
J.Orenstein et al Science 288, 468 (2000)



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
Solitonic lattices in spin-Peierls GeCuO in HMF - Grenoble

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 self-traping 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 into solitons.
- Continuously broken symmetries allow for solitons to enter D>1 world of long range ordered states: SC, ICDW, SDW.
- They 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

Some obligatory references :

Brinkman & Rice
Dzyaloshinskii & Larkin
Finkelstein & Wiegman
Fukuyama & Tanaka
Kirova
Kusmartsev
Luther & Emery
Matveenko
Mineev & Volovik
Nagaev
Schrieffer
Schultz
Shriman and Sigia
Varoquaux
Zaanen
etc., etc.