Peter Karpov and Serguei Brazovskii

MODELING OF PATTERNS IN ELECTRONIC CRYSTALS:

EFFECTS OF LONG-RANGE COULOMB INTERACTIONS FOR POLARONS AND

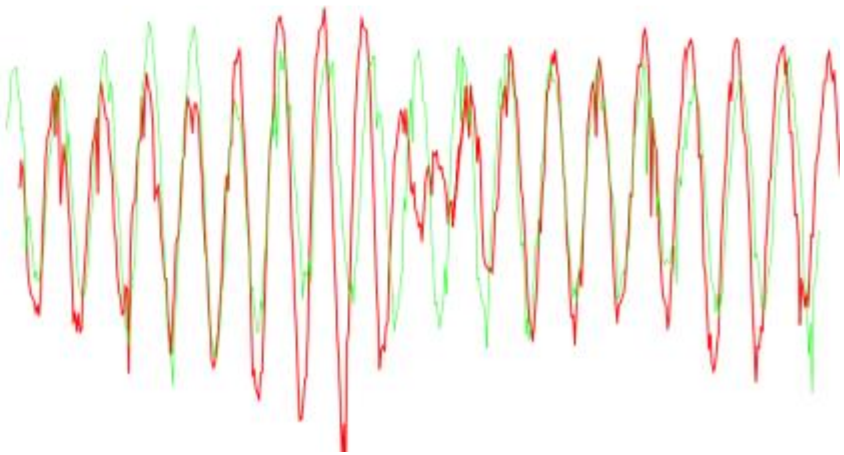
ALSO OF SUPER-LONG RANGE ONES FOR SOLITONS CONFINEMENT

PART I:
Pattern Formation and Aggregation In Ensembles of Solitons
in Quasi One-Dimensional Electronic Systems – combined symmetries.

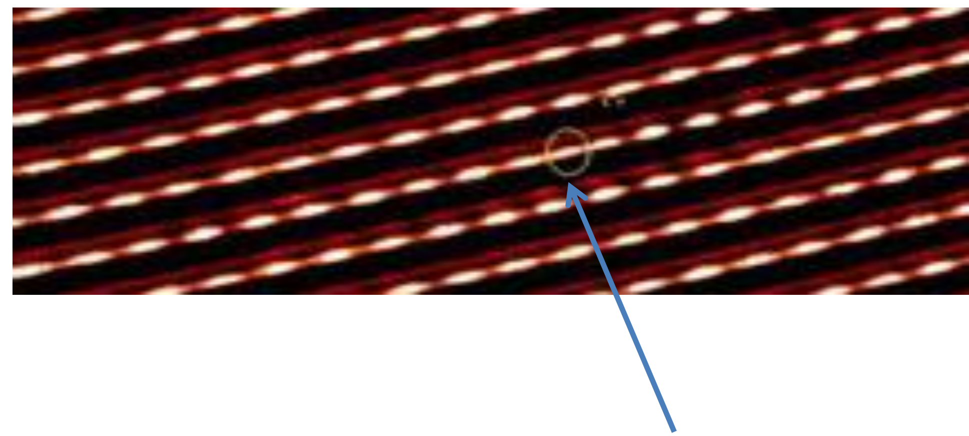
Applicable to incommensurate CDWs and SDWs (wait for N. Kirova talk),
FFLO in spin-polarized superconductors, holes in the AFM background.

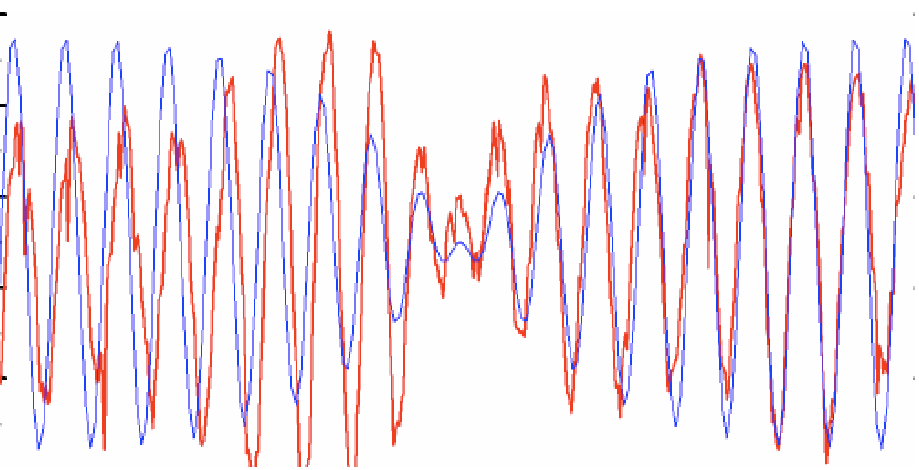
STM in NbSe3, Brun, Wang, Monceau & SB, PRL 2012

The CDW is perforated here and there by nodes of amplitude



Profile along the defected chain vs its nearest neighbor





Defected chain vs theory

$$-\tanh(x/\xi) * \sin(2\pi x/\lambda + \arctan(x/l))$$

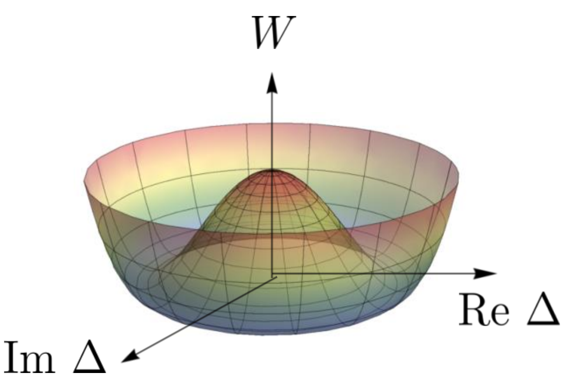
Phase stretching by π over long tails allows the amplitude kink to adapt to a long range 3D order. General concept: topologically bound complex of the kink core and the half-integer vortex.

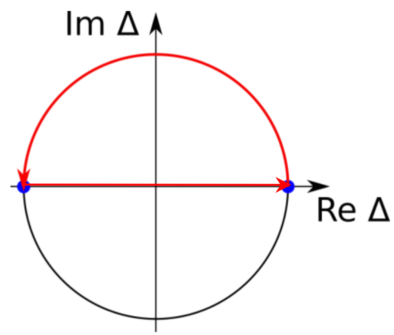
Discrete vs continuous degeneracy of the ground state

∞-degenerate ground state (incommensurate CDW)

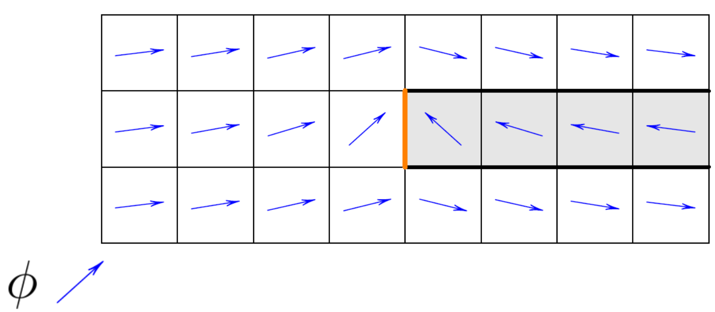
$$\rho(x) = \rho_0 + A(x)\cos(2k_F x + \phi(x))$$

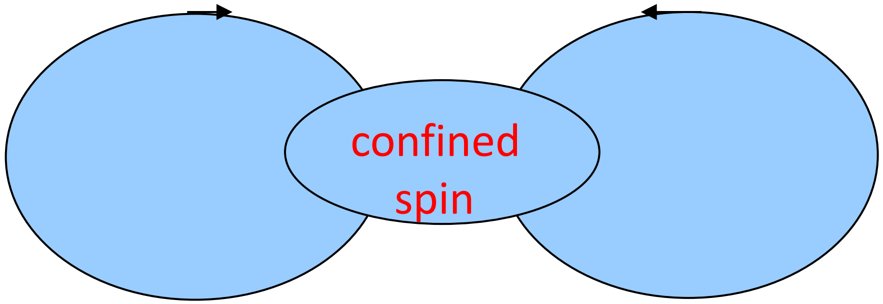
complex order parameter: $\Delta(x) = A(x)e^{i\phi(x)}$



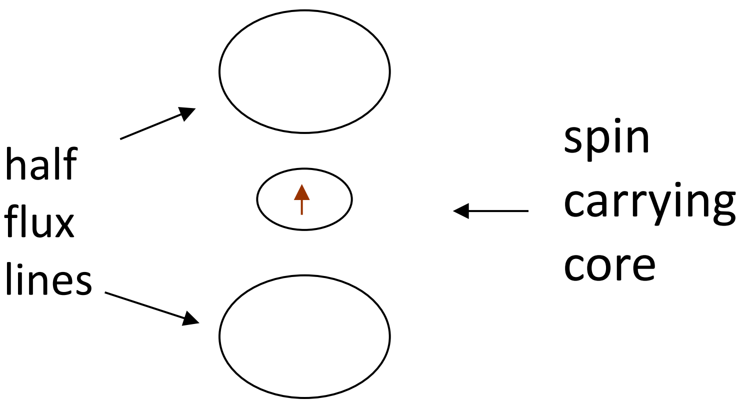


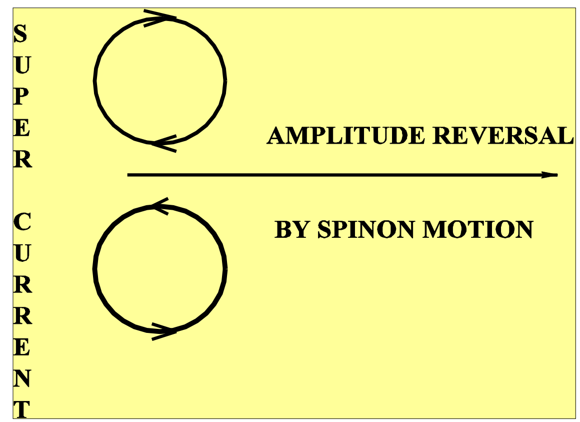
amplitude-phase soliton





Spinon as a soliton + semi-integer π-vortex of φ in a CDW or a SC



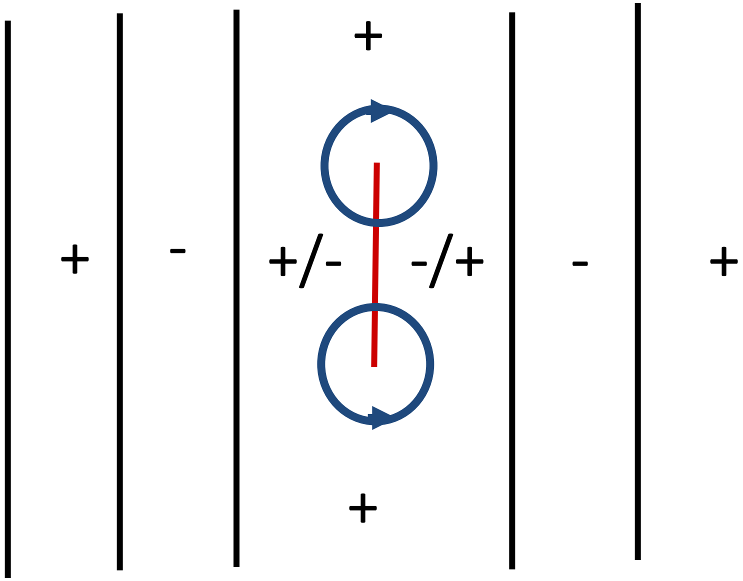


Quasi 1d view : spinon as a π- Josephson junction in the superconducting wire (*applications: Yakovenko et al*).

2D view : pair of π- vortices shares the common core bearing unpaired spin.

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

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



Kink-roton complexes as nucleuses of melted lattices: FFLO phase for superconductors or strips for doped AFMs. (*ref to L. Radzihovsky*)

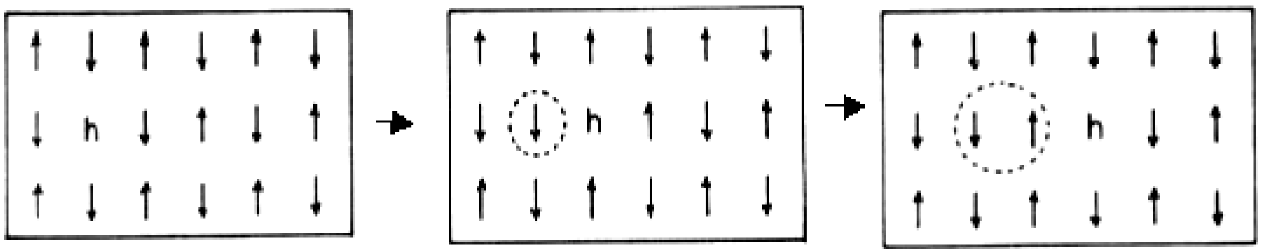
Defect is embedded into the regular stripe structure (black lines).
+/- are the alternating signs of the order parameter amplitude.

Termination points of a finite segment L (red color) of the zero line must be encircled by semi-vortices of the π rotation (blue circles) to resolve the signs conflict.

The minimal segment would correspond to the spin carrying kink.

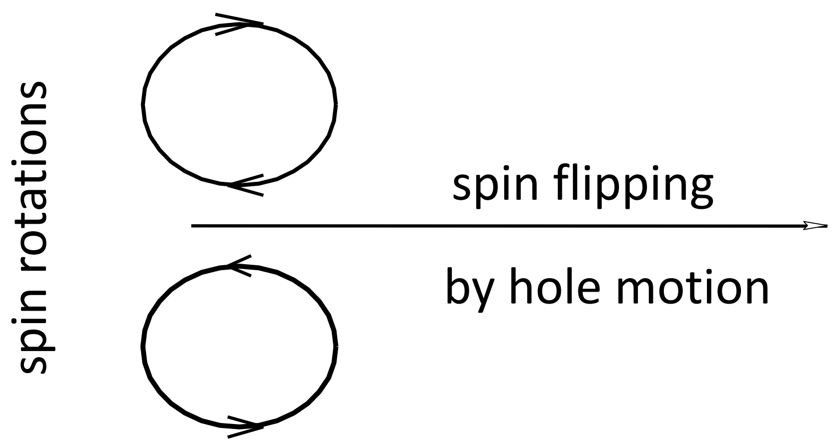
Propagating hole in a doped AFM state as an amplitude soliton.

Its motion permutes AFM sublattices ↑,↓
creating a string of the reversed order parameter:
staggered magnetization. It blocks the direct propagation.



Bulaevskii, Khomskii & Nagaev. Brinkman and Rice.

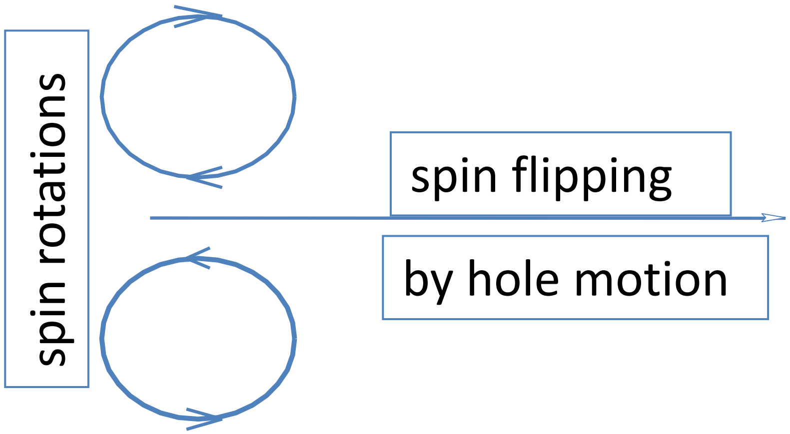
Adding the semi-vorticity to the string end heals the permutation thus allowing for propagation of the combined particle.



Alternative view:
Nucleus of the stripe phase or the minimal element of its melt.

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 - phase of charge displacements

θ - phase of spin rotations.

Degeneracy of the ground state:

$\varphi \rightarrow \varphi+\pi$ = translation by one site, gives a holon or doublon

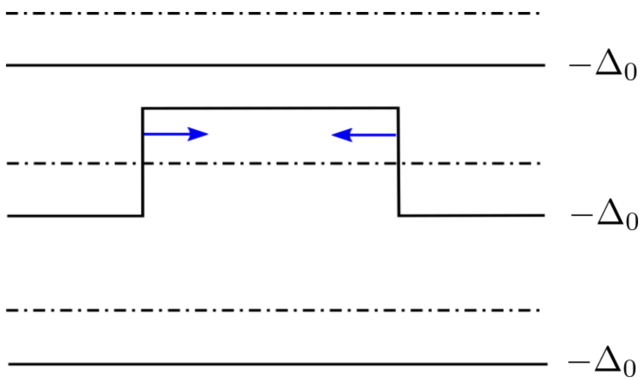
Staggered magnetization $\equiv$ *AFM=SDW order parameter:*

$O_{SDW} \sim \cos(\varphi)\exp\{\pm i(Qx+\theta)\}$, amplitude $A=\cos(\varphi)$ changes the sign

To survive in D>1 : The π soliton in φ : $\cos\varphi \rightarrow -\cos\varphi$ enforces a π rotation in θ to preserve O_{SDW}

Ensembles of solitons in D>1: pairwise confinement vs domain walls formation

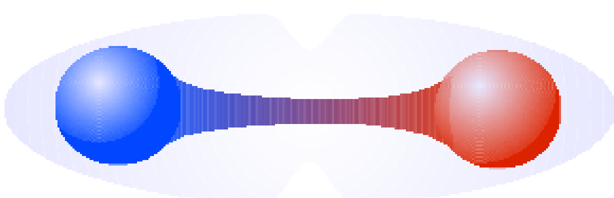
Solitons on one chain



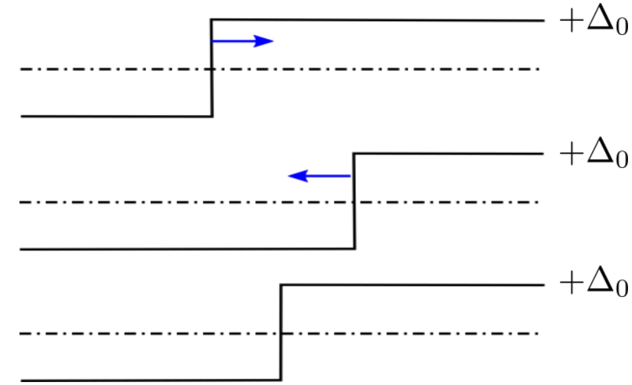
Forming the on-chain pairs = bisolitons

Pairwise binding at a higher $T=T_1$

Confinement!

q  $\bar{q}$

Solitons on different chains



Aggregation into transversal walls

↓

Stripes formation at a lower $T=T_2$

$$E \sim l,\ F = const$$

Effective classical model

Discretized classical variables:

α - chain index, i –in chain sites

$S_{i\alpha}$ =1,-1 Ising varible for the amplitude

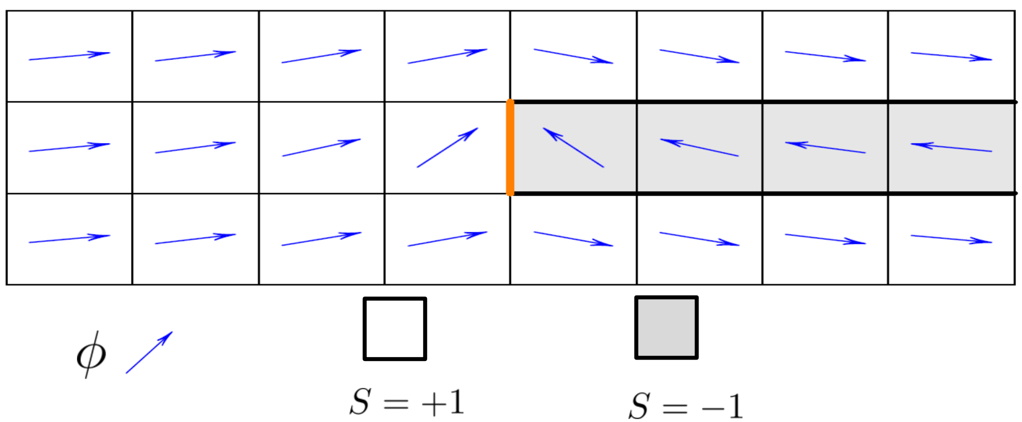
$\phi_{i\alpha}$ – phase variable

$\phi_{i,\alpha} = \langle \phi_\alpha(x_i) \rangle$ – XY-like (angle) variable

$$H = -J_{||} \sum_{i,\alpha} S_{i,\alpha} S_{i+1,\alpha} - A_{||} \sum_{i,\alpha} \cos(\phi_{i,\alpha} - \phi_{i+1,\alpha}) - A_{\perp} \sum_{i,\langle \alpha,\beta \rangle} S_{i,\alpha} S_{i,\beta} \cos(\phi_{i,\alpha} - \phi_{i,\beta})$$

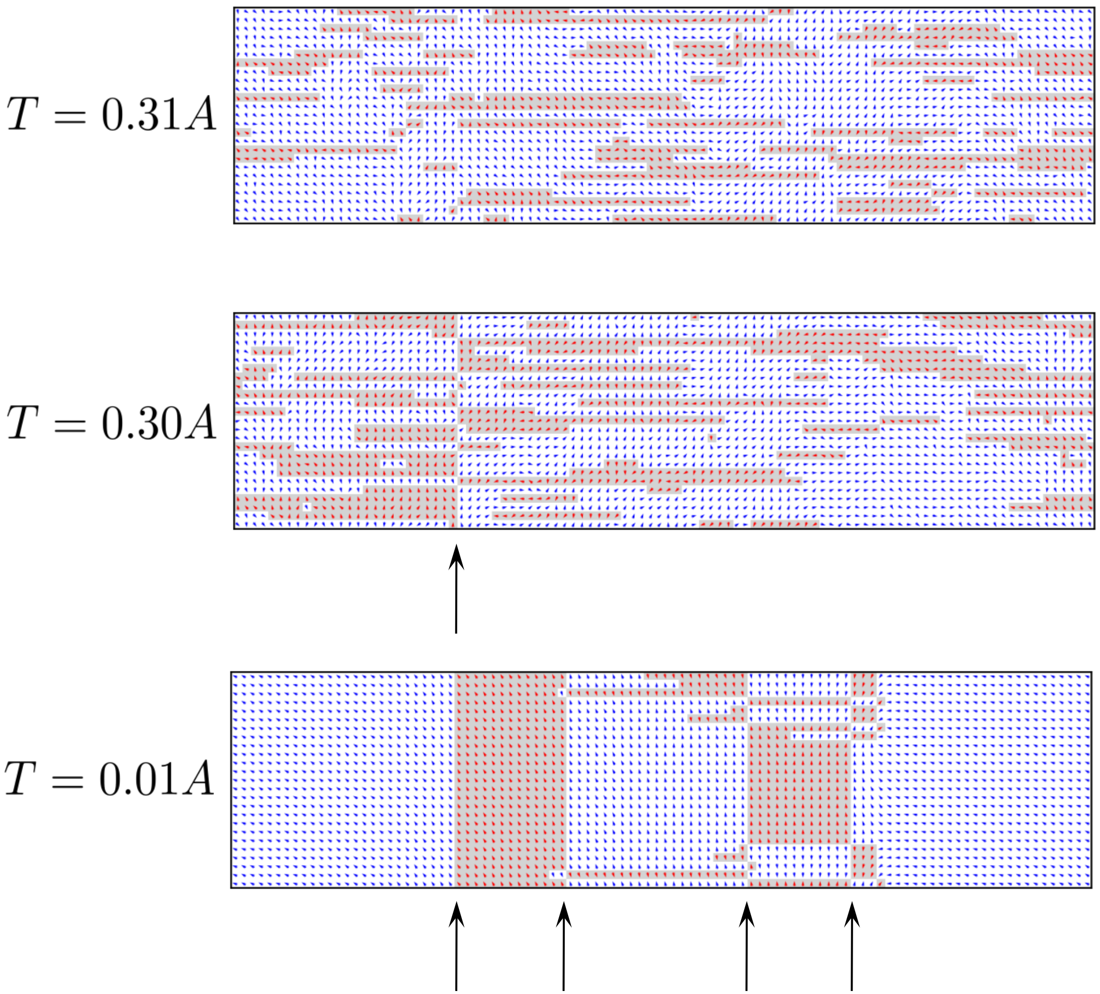
$$\begin{cases} S_{i,\alpha} \to -S_{i,\alpha} \\ \phi_{i,\alpha} \to \phi_{i,\alpha} + \pi \end{cases} \quad \text{for all } S, \phi \text{ at a given chain } \alpha$$

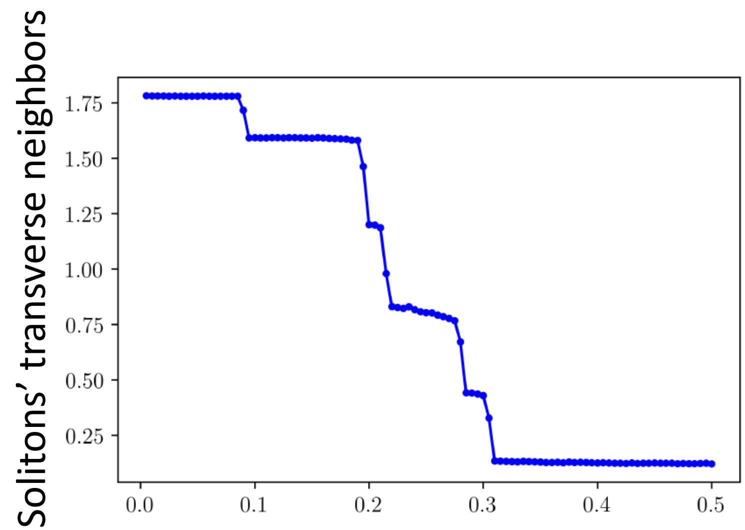
amplitude-phase soliton



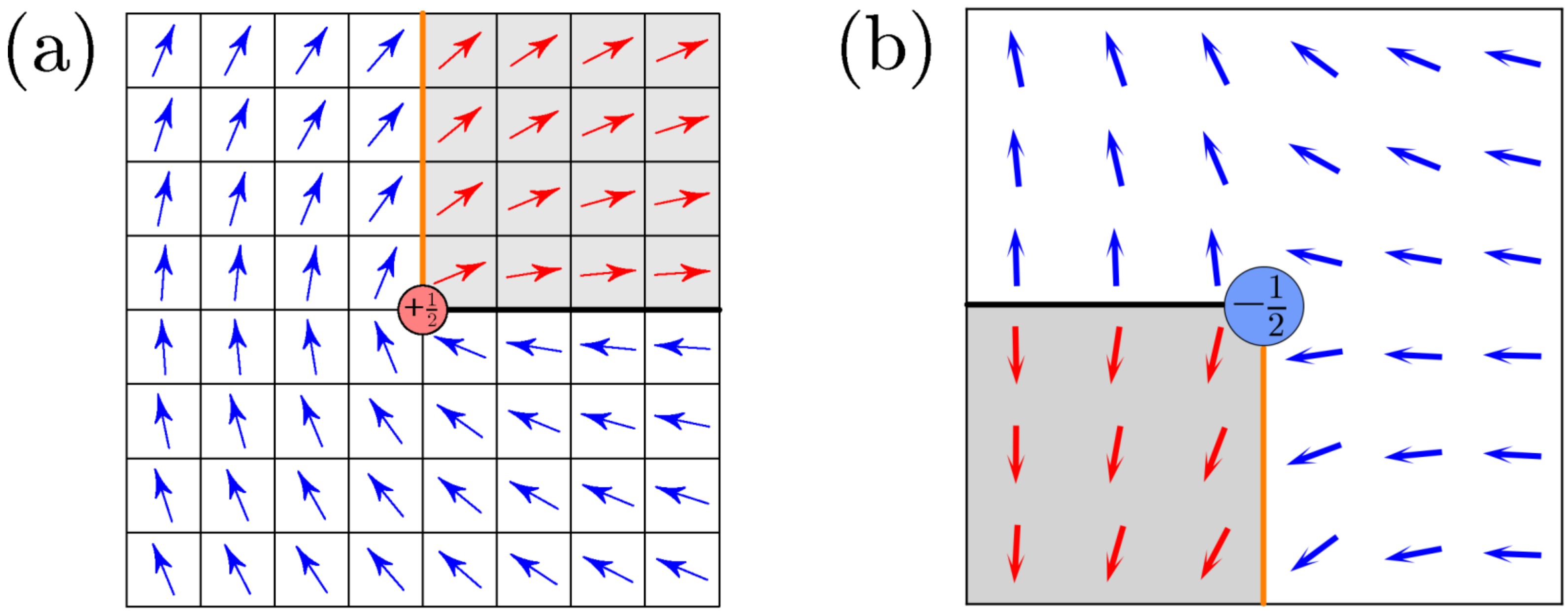
Monte-Carlo simulations throught two phase transitions:

1. Long range order which confines kinks with vortices.
2. Aggregation of confined complexes into extended walls.
3. Progressive multiplication of walls till the solitonic material is exhausted.

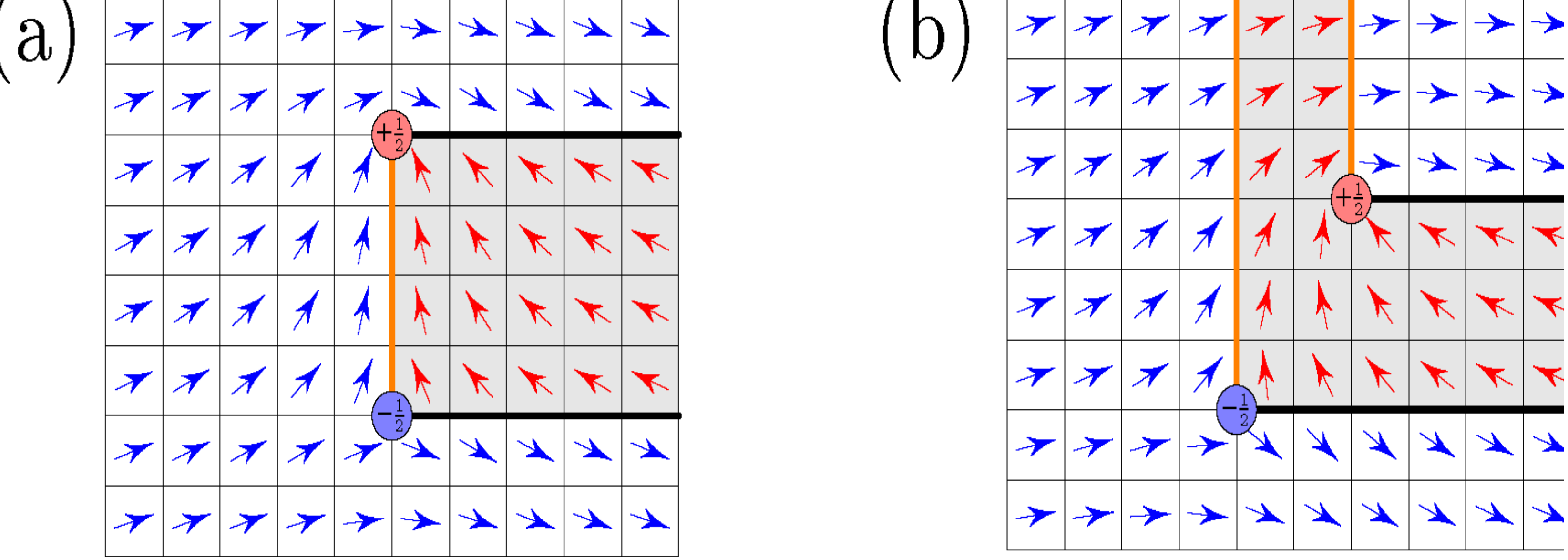




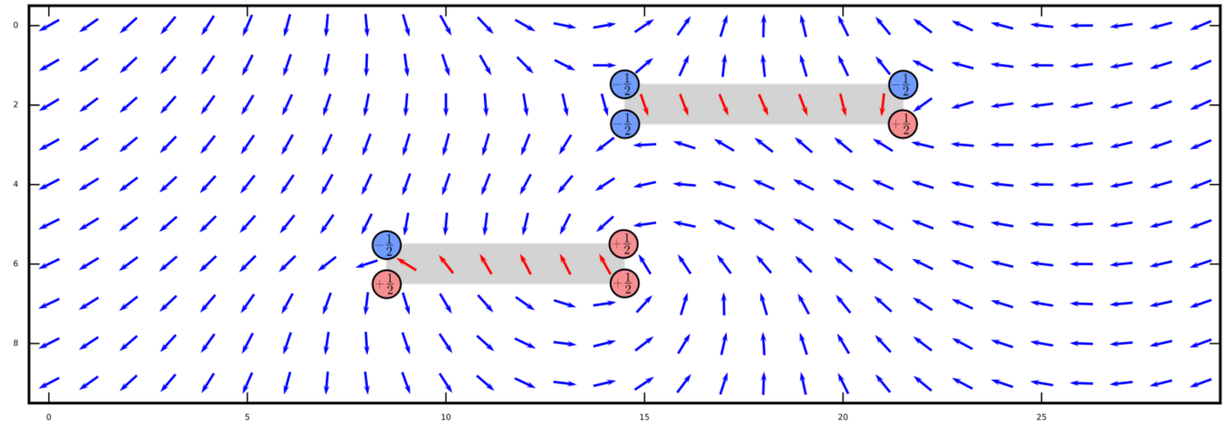
Types of topological cofigurations extracted from raw pictures for D=2:



Half-vortex (**a**) and half-antivortex (**b**).
Arrows: the rotational degree of freedom,
white/gray shading – amplitude sign,
orange (transverse to chains) line: the array of amplitude solitons,
black (along the chains) line: a string attached to a half-vortex.
disks: the cores of half-integer (anti)vortices.



Half-integer vortex-antivortex pairs.
(**a**) $T > T_2$, the pair structure is dominated by the linear confinement potential, solitonic walls (orange) are finite.
(**b**) $T < T_2$, the pair structure is dominated by pseudo-Coulomb BKT log-potential, solitonic walls grow to infinity.



Configurations with four solitons after a rapid quenching.

Broken symmetries of quasi one-dimensional electronic systems give rise to microscopic solitons taking roles of carriers of the charge or spin.

Continuous degeneracies for the complex order parameter gives rise to phase vortices, amplitudes solitons, and their combinations.

These degrees of freedom can be controlled or accessed independently via either the spin polarization or the charge doping.

The long-range ordering in dimensions above one imposes super-long-range confinement forces upon the solitons, leading to a sequence of phase transitions in their ensembles.

Higher-T transition enforces the confinement of solitons into topologically bound complexes: the amplitude solitons dressed by exotic half-integer vortices.

At a lower T transition, solitons aggregate into into walls terminated by rings of half-integer vortices.

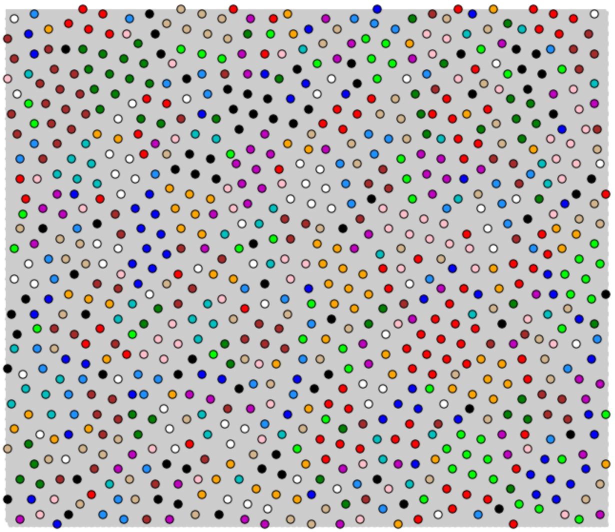
With lowering T, walls multiply, passing sequentially across the sample.

The efficient Monte Carlo algorithm, preserving the number of solitons, facilitated calculations, extending them to the 3D case and including the long-range Coulomb interactions.

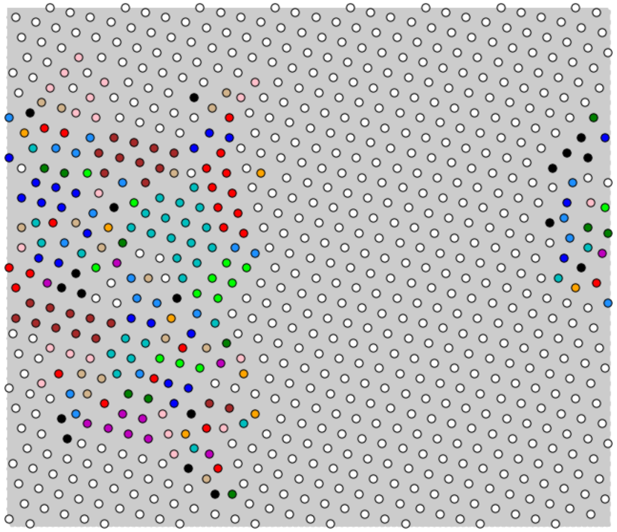
PART II, FORMATION AND EVOLUTION OF DOMAIN WALLS' GLOBULES AND NETWORKS SIMULATED FROM A MODEL WITH ONLY COULOMB REPULSION

Model definition: basis of a regular (hexagonal here) crystal of **N** sites.
Seed **M** charges with a concentration close to the one allowing them to form a regular superlattice minus **n** holes **(M=N-n)/13** here).
Impose Coulomb repulsion; proceed Monte-Carlo cooling.

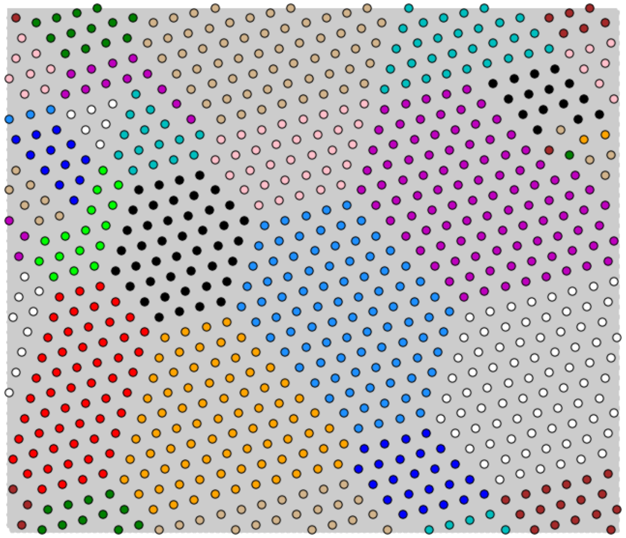
Evolution from high temperatures through the phase transition. **n= 12**
Colors indicate different ways to form the sublattice: 26'th degeneracy



High T, no LRO, defects and regular sites are not distinguishable



Just below the 1st order transition. Cloud of defects within a single LRO domain.

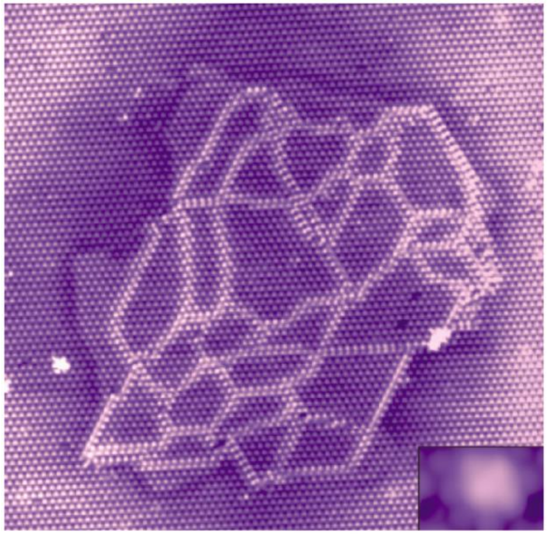


The relaxed defects build a network of domain walls framing a mosaic polycrystal.

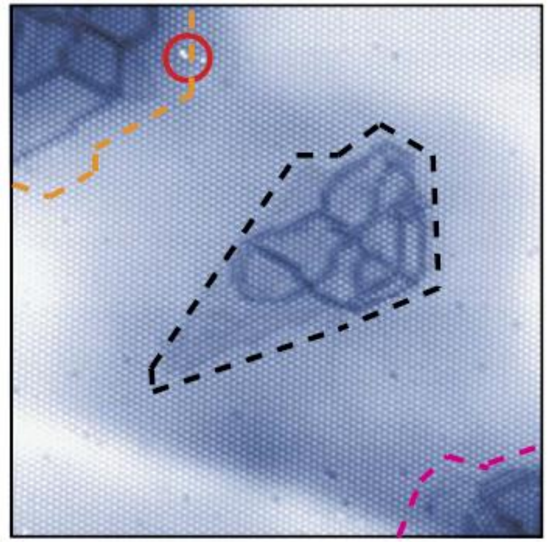
Modeling vs experiments: low doping

experiment

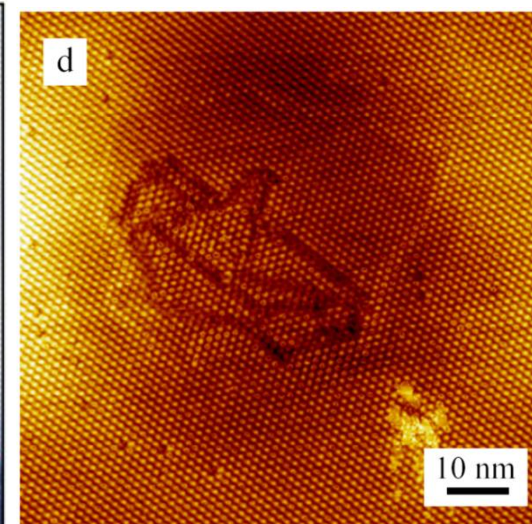
Ma et al (2016)



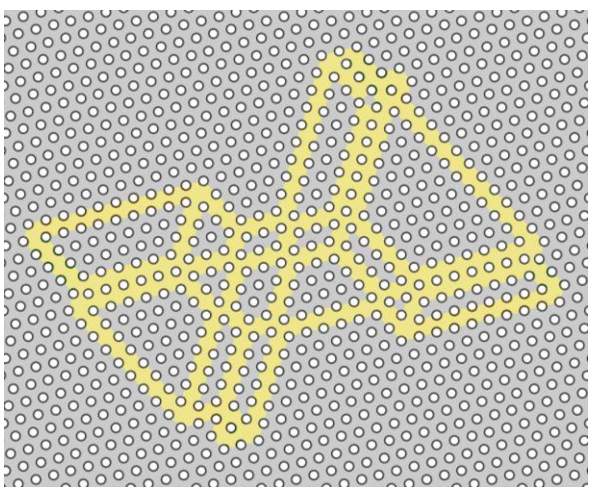
Cho et al (2016)

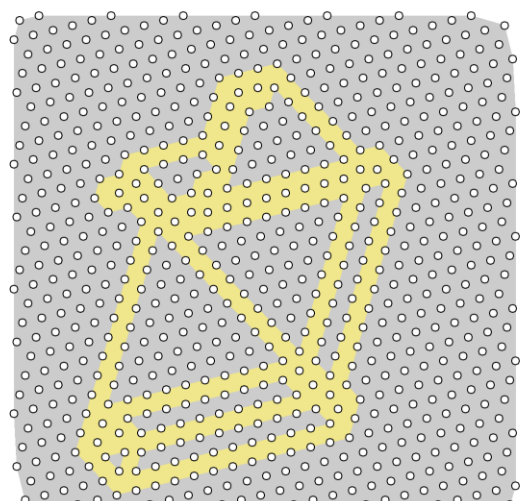


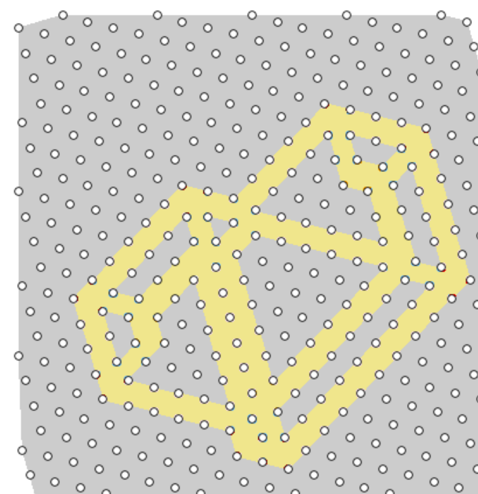
Vaskivskyi et al (2016)



$\nu_{voids} \approx 1\%$







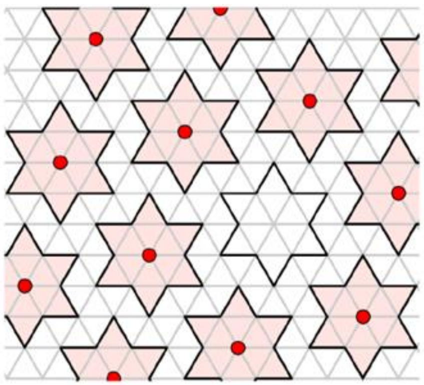
modeling

Globules of domain walls

How comes that LR Coulomb repulsion allows charges to aggregation ?

Common guesses: local energy gains from striction, exchange, etc.

Void vs domain wall which are due to the multiple symmetry breaking

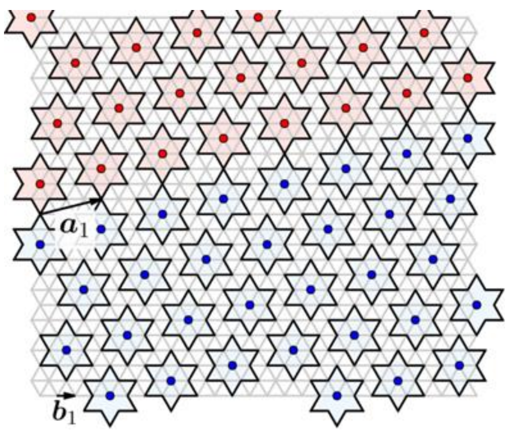


a

Single void

$$E_{void} \simeq \frac{e^2}{a}$$

One-step wall with the same charge $+e$



$$E_{wall} \simeq 13 \int_a^\infty \frac{(e/13)^2}{r} \exp(-r/l_s) \simeq \frac{\ln(l_s/a)}{13} \times \frac{e^2}{a}$$

$q = +e/13$ per a_1

Charge fractionalization → energy gain!

The minimalistic statistical model allows to resolve the **seeming paradox**: **why charged voids aggregate instead of diverging?**

The apparently surprising behavior indicates that some effective attraction develops from the purely repulsive Coulomb interactions.

Wall's formation is not gust gluing of holes but their fractionalization.

The domain wall is fractionally (**q=en/13, n=1,…**) charged thus reducing the Coulomb self-energy versus the integrally charged (**q=e**) single hole.

Being still the charged lines, the domain walls repel each other but as topological objects they can terminate only at points of the triplet branching, thus forming the connected globes.

Fractionally charged walls cannot further disintegrate because of their topological nature: they connect different degenerate ground states.