Combined fractional charge-spin vortices in spin density waves

Natasha Kirova

Laboratoire de Physique des Solides,

CNRS & Université Paris-Saclay, Orsay, France

QRC, Skolkovo, Russia

Collaboration:
S. Brazovskii *LPTMS, CNRS &*
Université Paris-Saclay, Orsay, France

Landau Week 2023, Erevan,
26/06/2023

Outline

- Introduction.

- Combined symmetry breaking and multiple topological defects in spin density waves (SDW).
- Phase, magnetic, and complex non-integer vortices.
- Spin anisotropy and confinement of vortices
- Narrow band noise (NBN) from phase slipes – instantons
- Related objects: hole motion in a dopped antiferromagnet, combined solitons
- Conclusions

Our interest lies in richer incommensurate superstructures:
charge density waves (CDW), spin density waves (SDW), Wigner crystals
Typically they are weak, almost sinusoidal superstructures $\propto \cos(Qx+\varphi)$
They possess a complete translational degeneracy exposed by the arbitrary displacement of the phase φ.
There are common features of incommensurate CDWs, SDWs, WCs related to their phase φ degree of freedom:
complex order parameters $\eta = A \exp[i\varphi]$, $\eta = A\mathbf{m} \exp[i\varphi]$
collective charge $n_c \sim \partial_x\varphi$ and current $j_c \sim -\partial_t\varphi$ densities
Phase increment $\Delta\varphi/2\pi$ controlling the number of condensed fermions

Observable collective effects related to the phase φ degeneracy

- Fröhlich conduction by the collective sliding $\varphi \propto \mathbf{t}$.
- Topological defects: solitons, dislocations (electronic vortices).
- Phase slips = instantons = spacio-temporary vortices
- Conversion among normal and condensed electrons by winding of the phase increment over the sample

Common peculiarity of DWs: Coulomb hardening, anomalous elastic theory and strong confinement of phase vortices

Energetics of dislocations is determined by strong Coulomb forces limited only by screening facilities of free carriers which freeze out at low T.

Linear approximation, constant amplitude, exclude electric potential and carriers,Fourrier representation φ_k and $ik_{\parallel}\varphi_k$ for the phase and the charge

$$W\{\varphi\} = \frac{\hbar v_F}{4\pi}\sum|\varphi_k|^2\left[\rho_c k_{\parallel}^2 + C_{\perp}{k_{\perp}}^2 + \frac{\rho_c^2 {r_0}^{-2} k_{\parallel}^2}{k_{\parallel}^2 + {k_{\perp}}^2 + {r_{scr}}^{-2}}\right]$$

$r_0 -$ short screening length in the parent metal

${r_{scr}}^2 = {r_0}^2/\rho_n$ – the acual long screening length in the DW

ρ_c, ρ_n=1-ρ_c condensate and normal carriers densities.

$\rho_n \rightarrow$1 at T $\rightarrow$T$_c$ and $\rho_n \sim \exp(-\Delta/T)$ vanishes at low T

$C_{\parallel}^0 = \rho_c$ and $C_{\perp} \sim A^2$ - compression and shear moduli

$r_\perp < r_0$: Coulomb interaction is not important standard elastic theory conventional energy for the pair of dislocations at a

$r_\perp = R_\perp$

$$W_{disl} = T_c ln(R_\perp/a_\perp)$$

$$W\{\varphi\} \approx \frac{\hbar v_F}{4\pi}\sum |\varphi_k|^2 \left[\rho_c k_\parallel^2 + C_\perp k_\perp{}^2\right]$$

$r_\perp \gg r_{scr}$: Coulomb interaction is screened, qualitatively a normal elastic theory but in stretched coordinates $(x\sqrt{C_\perp \rho_n/\rho_c}$, $r_\perp)$ which inclination diverges at low **T**

$$W\{\varphi\} \approx \frac{\hbar v_F}{4\pi}\sum |\varphi_k|^2 \left[(\rho_c/\rho_n)\, k_\parallel^2 + C_\perp k_\perp{}^2\right] \qquad C_\parallel = \rho_c/\rho_n$$

Again the logarithmic vortex energy but with the energy scale greatly enhanced as $\mathbf{r_{scr}/r_0=1/\sqrt{\rho_n}}$

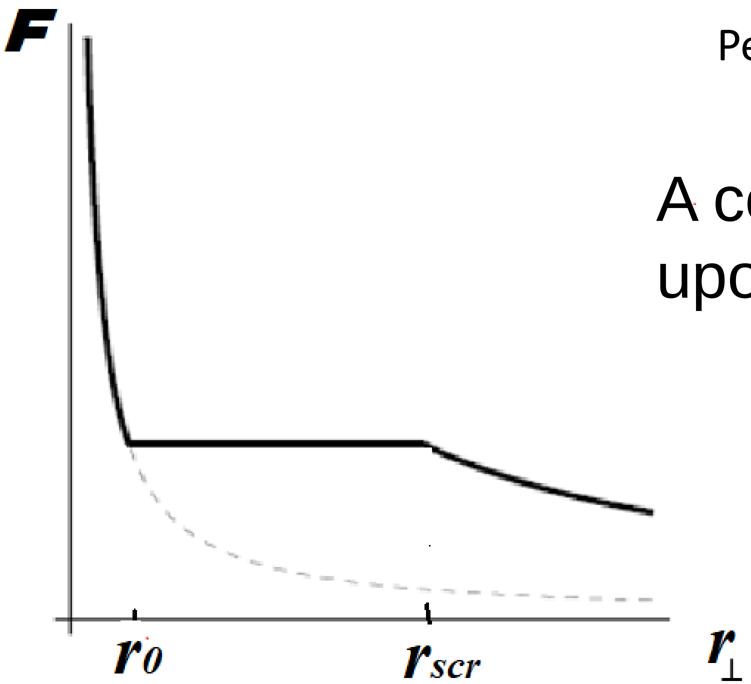
$$W_{disl} = T_c \frac{r_{scr}}{r_0} ln(R_\perp/r_0) = T_c \frac{1}{\sqrt{\rho_n}} ln(R_\perp/r_0)$$

$$r_0 < r_\perp < r_{scr}:$$

nonlocal elastic theory with energy dependent on ratio of gradients rather on their values

$$W\{\varphi\} \approx \frac{\hbar v_F}{4\pi} \sum |\varphi_k|^2 \left[\rho_c k_\parallel^2 + C_\perp {k_\perp}^2 + \frac{{r_0}^{-2} k_\parallel^2}{{k_\perp}^2} \right]$$

Curious confinement law is with $\boldsymbol{W_{disl} \sim T_c (R_\perp / r_0)}$



Perimetric instead of logarithmical law.

A constant force ***F*** acting upon the D-line

Order parameter and allowed topological defects $\eta \to \eta$

CDW

η_{CDW}=Aexp(i**Qr**+ φ)

$\rho_{CDW} = |\eta_{CDW}| \cos(Qx+\varphi)$

- Phase vortex, dislocation, 2π translation:
  $\varphi \to \varphi + 2\pi$
- Amplitude soliton : φ=const
- combined object :

amplitude-phase soliton

$\varphi \to \varphi+\pi$, A =-1$\to$A=+1

SDW

m is the unit vector of the staggered magnetization

η_{SDW}=A**m**exp(i**Qr**+ φ)

$\rho_{SDW} = |\eta_{SDW}|^2 \cos(2Qx+2\varphi)$

- Phase vortex, dislocation, 2π translation:

$\varphi \to \varphi+2\pi$, **m**$\to$**m**

- normal **m** - vortex, 2π rotation:

m$\to O_{2\pi}$ **m**, $\varphi \to \varphi$

- combined object :

$\varphi \to \varphi+\pi$, **m**$\to O_{\pi}$ **m** = **-m**

Phase vortex and magnetic vortex

Energy of the vortex with the winding number ***z***: $W_m \sim T_c \rho_s \boldsymbol{z^2}$

Energy of the dislocation (***z =1***) : $W_\varphi \sim T_c(\rho_s/\rho_n)z^2$

In general if $\boldsymbol{z \to 2(z/2)}$ then $W \to W/2$

Only smallest z are stable

T~Tc : $W_\varphi \sim W_{\mathbf{m}}$ all energies are comparable

- Normal dislocation
- Half-dislocation combined with semi-vortex
- Normal magnetic vortex

Result depends on numbers.

T<<Tc : $W_\varphi \gg W_{\mathbf{m}}$

- Half-dislocation combined with semi-vortex –
- ***obligatory decoupling of the dislocation***

$\nu_\varphi = 1 \to \nu_\varphi = 1/2,\ \nu_m = 1/2$

$\nu_\varphi = 1 \to \nu_\varphi = 1/2,\ \nu_m = 1/2$

$\to$ **$W = (W_\varphi + W_m)/2 = W_\varphi/2$**

Modeling of topological defects in a SDW. Energy functional for a planar SDW *m={cos θ , sin θ}*

$$F=\int dx\,dy\left[\begin{array}{c}\frac{C}{2}\left(A^2-1\right)+\frac{K_{Ax}}{2}(\partial_x A)^2+\frac{K_{Ay}}{2}\left(\partial_y A\right)^2+\frac{1}{\pi}A^2\Phi\partial_x\varphi\\ -HA^2\partial_x\theta+\frac{K_{\varphi x}}{2}(\partial_x\varphi)^2+\frac{K_{\varphi y}}{2}A^2\left(\partial_y\varphi\right)^2\\ +\frac{K_{\theta x}}{2}A^2(\partial_x\theta)^2+\frac{K_{\theta y}}{2}A^2\left(\partial_y\theta\right)^2+F(n,A)\end{array}\right]$$

$$F(n,A)=n^2/(2N_F)+(-\tau+(n/n_{cr})^2)(A\Delta_0)^2N_F/2+bA^4\Delta_0^2N_F/4$$

Charge and charge current condensate densities

$$\pi n_c=A^2\partial_x\varphi \qquad \pi j_c=-A^2\partial_t\varphi$$

Spin and spin current condensate densities

$$\pi n_s=A^2\partial_x\theta \qquad \pi j_s=-A^2\partial_t\theta$$

Problem of choosing variables for the numerical modeling.
The energy, density, current are simple and transparent in variables of the amplitude and the phase. But for vortices the phase is not uniquely defined which prevents their appearance in calculations. E.g. for a CDW the non-invariant but unique pair **{u,v}** has to be used: $\mathbf{\Psi=u+iv}$ rather than $\mathbf{\Psi=A\exp(i\varphi)}$
For a planar SDW, with m={cosθ,sinθ} the natural choice seems to be the spherical vector for the 3-degrees of freedom

We should use the spherical vector for the 3-degrees of freedom

$$\boldsymbol{\Psi} = Ae^{i\varphi}\{cos\theta, sin\theta\} \rightarrow$$

S=$\{u, v, w\} = \{A\ sin\theta\ cos\varphi,\ A\ sin\theta\ sin\varphi,\ A\ cos\theta\}$

$$\boldsymbol{\Psi} = (u + iv)\left\{\frac{cos\theta}{sin\theta}, 1\right\} = (u + iv)\left\{\frac{\pm w}{\sqrt{u^2 + v^2}}, 1\right\}$$

$$A^2 = u^2 + v^2 + w^2 \qquad cos\theta = \frac{w}{A}; \quad tan\varphi = \frac{v}{u}$$

$$\partial\varphi = \frac{u\partial v - v\partial u}{u^2 + v^2} \qquad \partial\theta = \frac{w(u\partial u + v\partial v) - \left(u^2 + v^2\right)\partial w}{A\sqrt{u^2 + v^2}}$$

Quite difficult for computations expressions still are not sufficient. The sign of $\boldsymbol{sin\theta}$ is not unique, notice $\pm\boldsymbol{w}$, preventing vortex configuration.

We were forced to use a more complex quaternion representation

$A\mathbf{m}\exp(i\varphi) = (u + iv)\{p, q\}$.

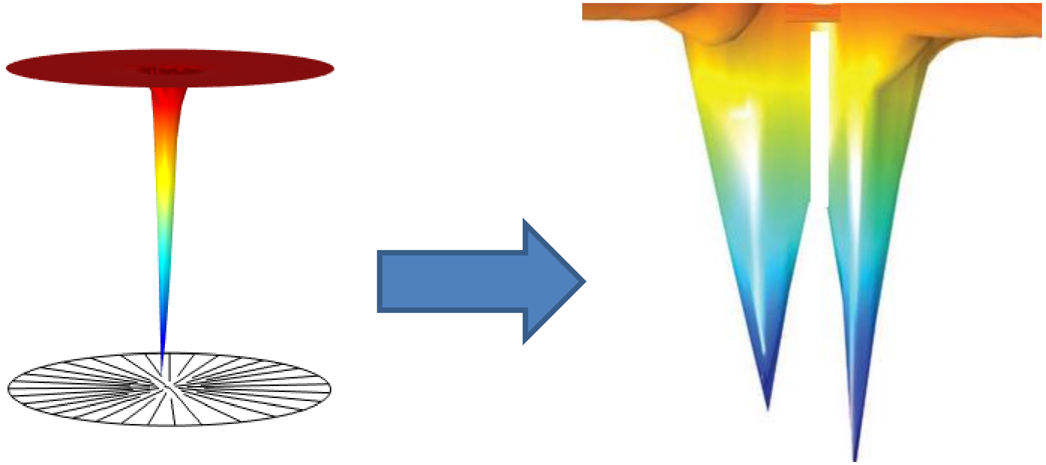
An over-complete set of four bilinear combinations
***{f, g, h, j}* = {*up, uq, p, q*}** imposing the apparent constant **fh = gj**.

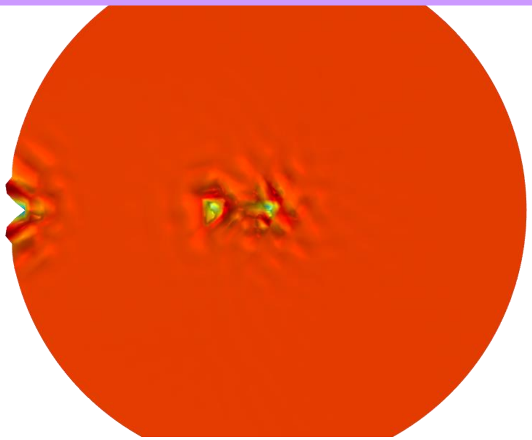
$$\boldsymbol{A^2 = f^2 + g^2 + h^2 + j^2}$$

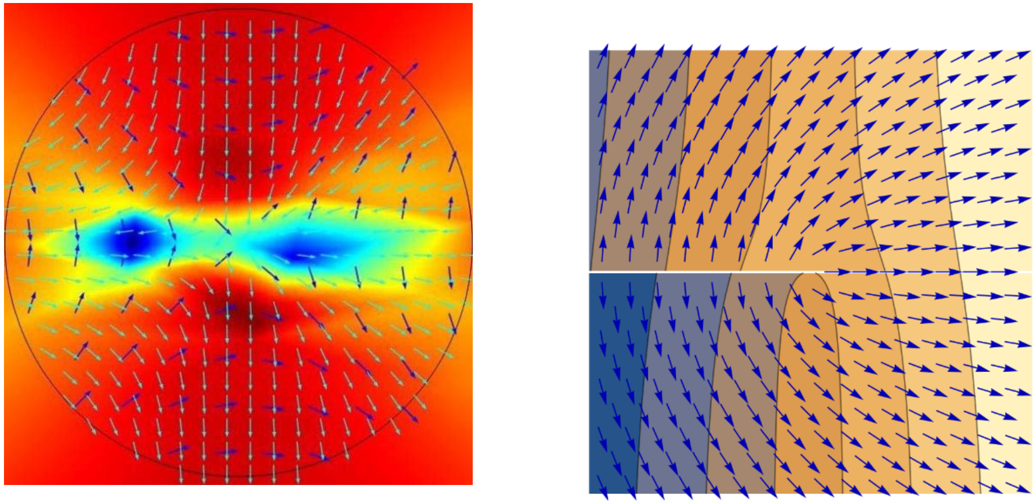
$$\boldsymbol{tg\varphi = h/f}; \quad \boldsymbol{ctg\theta = h/j}$$

It yields even more ugly expressions for derivatives and, worse, the constraint which adds a time-independent equation preventing facilities of efficient Cauchy's t algorithms in favor of more cumbersome finite element methods.

SDW: modeling for splitting of one charge vortex = dislocation into two combined vortices (chimers of half-spin+half-charge)







The vector field of the local SDW magnetization for the a chimer.
The chain axis is horizontal.

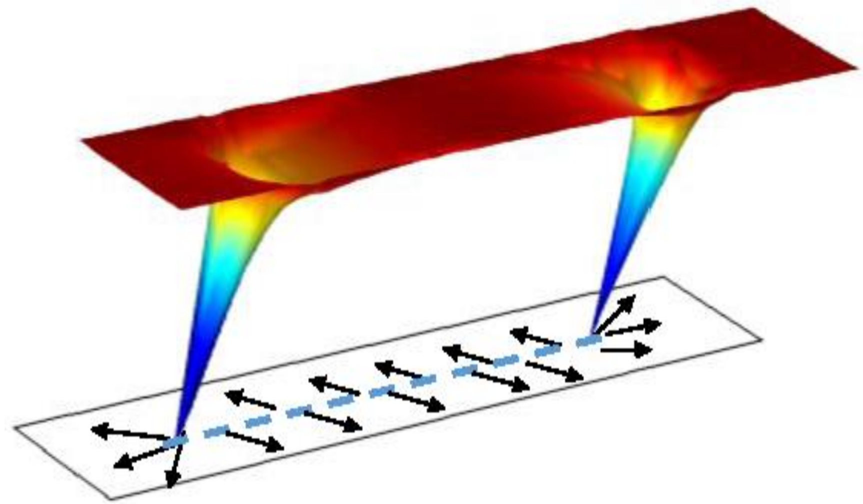
Spin – orbital coupling (Anisotropy)

Spin anisotropy costs diverging energy. That confines any spin vortex to the domain walls.

$W_m \sim (\partial_i m_\alpha)^2 + l^{-2}\, m_z^2$]

l - the wall's width

π semi-vortex $\rightarrow$ 180^o domain wall



The two π phase vortices will be bound by a string - the Neel domain wall.

With known parameters, the string length may reach the sample width.

Coulomb deconfinement against anisotropy confinement

Splitting of the **2π** phase vortex into two half-dislocations bound by the string of the180^o domain wall

$r<r_{scr}$: Energy lost $W_m = W_{wall} N$, N – distance in chains number

Energy gain $W_{Disl.} = -E_0 N/2$, $W_{wall} << E_0$

$E_0 > W$ - ***constant repulsion wins against constant attraction***

$r>r_{scr}$: Energy lost : $W_m = W_{wall} N$

Energy gain : $W_{Disl.} = -(E_0/2\rho_n^{1/2}) \ln N + W_{wall} N$

Equilibrium distance between half dislocations

$$N \sim E_0/(\rho_n^{1/2} W_{mDW})$$

$\rho_n^{-1/2}$ factors – recall the Coulomb hardening

Narrow Band Noise Generation

Sliding Charge/Spin Density Waves generate the Narrow Band Noise (NBN) - a coherent periodic unharmonic signal with the fundamental frequency Ω being proportional to the mean dc sliding current j with the universal (in CDWs) ratio Ω /j =π.

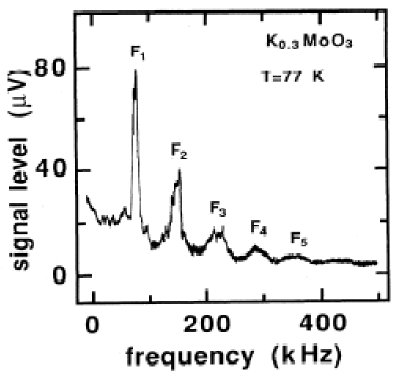


FIG. 1. Narrow-band noise spectrum from a thin sample of $K_{0.3}MoO_3$ at $T = 77$ K.

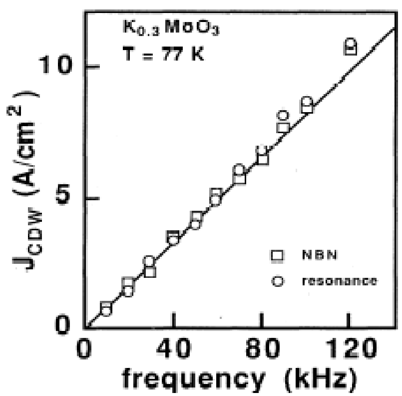


FIG. 8. The CDW current density at resonance plotted as a function of the resonance frequency (circles). The CDW-current-density-to-NBN-frequency (f_{NBN}) ratio is also plotted in the figure (squares).

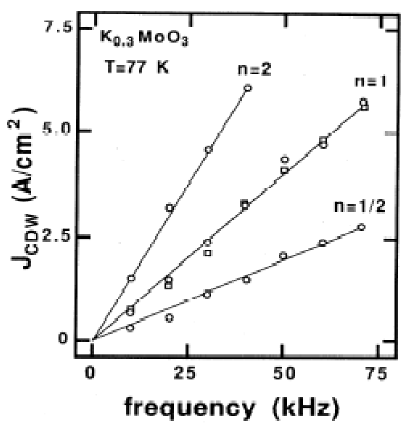


FIG. 5. CDW current density plotted as a function of external locking frequency for both Shapiro-step data (circles) and narrow-band-noise data (squares).

Realization of real time instantons - phase slips (x,t) sequence

CDW : ρ_{CDW} =A cos(Qx+φ); Ω /j= π.

Competing models:

The Wash-Board Frequency (WBF) model : NBN is generated *extrinsically* while the DW modulated charge passes through the host lattice sites or its defects.

But :

(i)The interaction between the rigid DW and the regular host lattice $V_{host} \sim \cos(Qx+n\Omega t)$, (usually $n=4$) $\rightarrow$ an n-fold WBF **contrary to experiments.**

(ii)Interaction with the host impurities $V_{imp} \sim \cos(Qx_i + \Omega t)$

the positionally random phase shifts $-Qx_i$ prevent any coherence in the linear response **Problem of space synchronization**

CDW $\rho_{CDW} = |\eta_{CDW}| \cos(Qx+\varphi)$ $\Omega/j = \pi.$

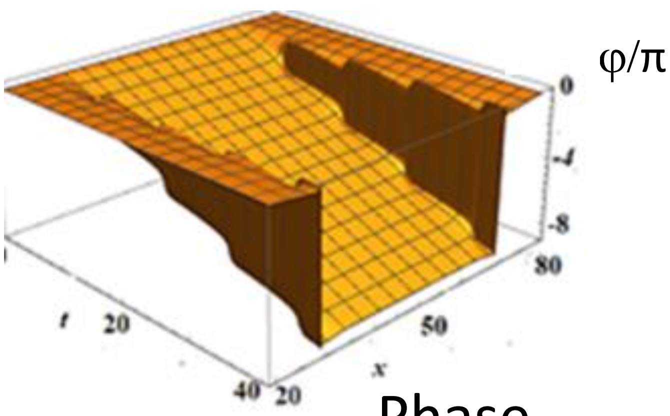
SDW $\rho_{SDW} = |\eta_{SDW}|^2 \cos(2Qx+2\varphi)$ $\Omega/j = 2\pi.$

***Phase Slip Generation (PSG) model*: **the NBN is generated by the phase slips occurring near injecting contacts.

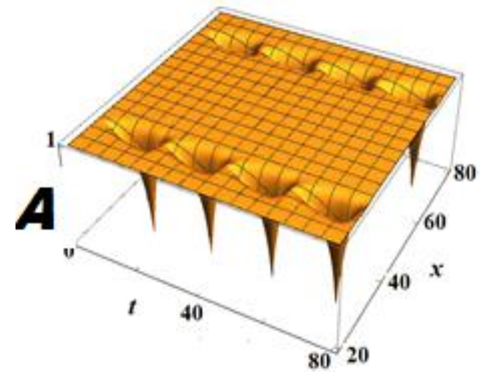
An old question of time synchronization

Our modeling confirms a regularity as shown by a remarkably high coherence of the NBN in experiments

DW does not slide at the sample side surface, coupling $\cos(\phi_{bulk} - \phi_{surface})$ with $\phi_{bulk} \propto t$ and $\phi_{surface} = cnst$ provides a necessary WBF. Bridge to our PSG modeling with constant boundary conditions.



Phase

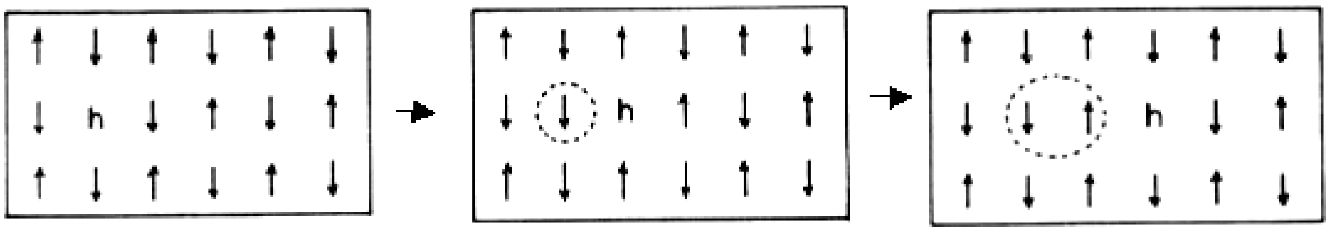


Amplitude

Our point of view: **Contrary to CDW the fundamental ratio NBN frequency to DC current is not the universal parameter**, changing from ½ near Tc to 1 at T<< Tc and being restorted to ½ in case of magnetic anisotropy.

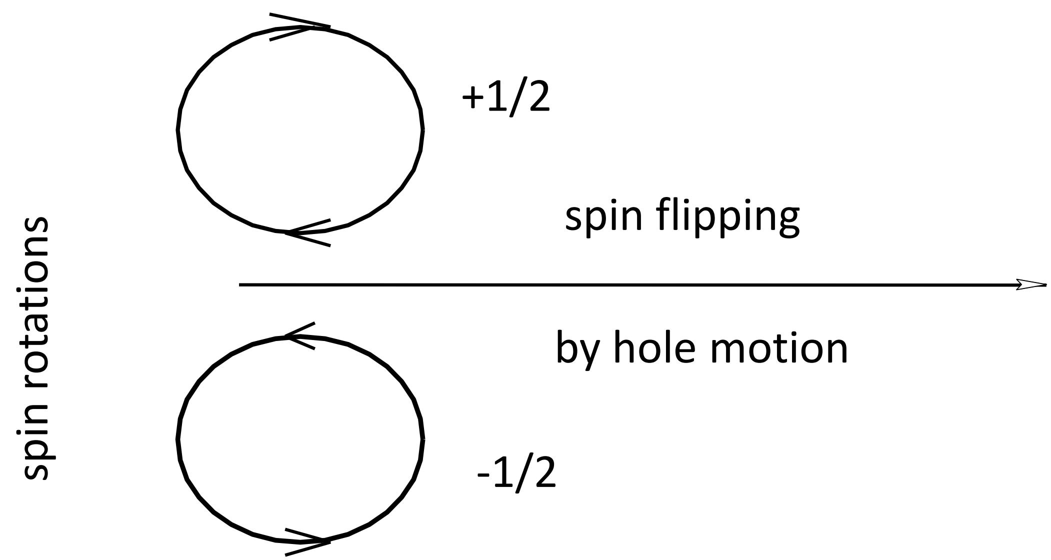
Related systems I. hole in the antiferromagnetc AFM environment

The motion permutes AFM sublattices ↑,↓ creating a string of the reversed order parameter: staggered magnetization. The lost interaction energy with neighboring lines grows linearly – the string blocks the hole propagation (the modern “fraction”).



Bulaevskii, Khomskii, Nagaev. Brinkman and Rice.

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



Related systems II : SDW route to the doped Mott-Hubbard insulator.

Quasi 1D, half filled band with repulsion, gap in charge phase, free spin phase, bosonization language.

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

U - Umklapp amplitude

φ - chiral phase of charge displacements

θ - chiral phase of spin rotations.

Degeneracy of the ground state:

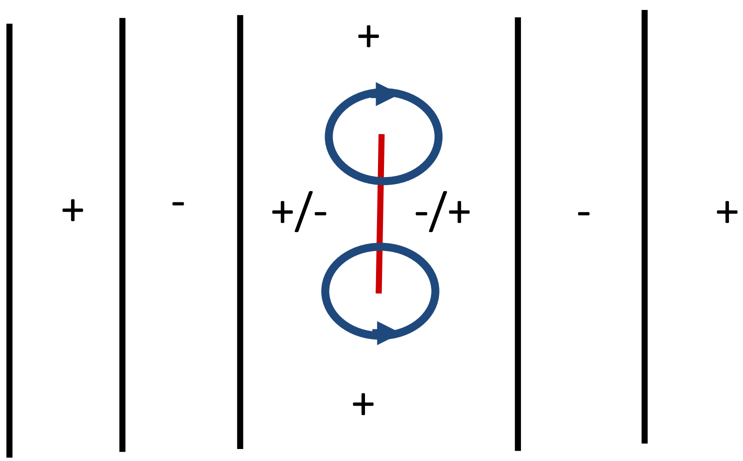
$\varphi \rightarrow \varphi+\pi$ = translation by one site

Staggered magnetization AFM=SDW order parameter:

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

Related systems III : Singlet systems: half-integer vortices in a superconductor SC with a partial spin polarization – FFLO phase of stripes with alternating signs of the amplitude of the SC order parameter.

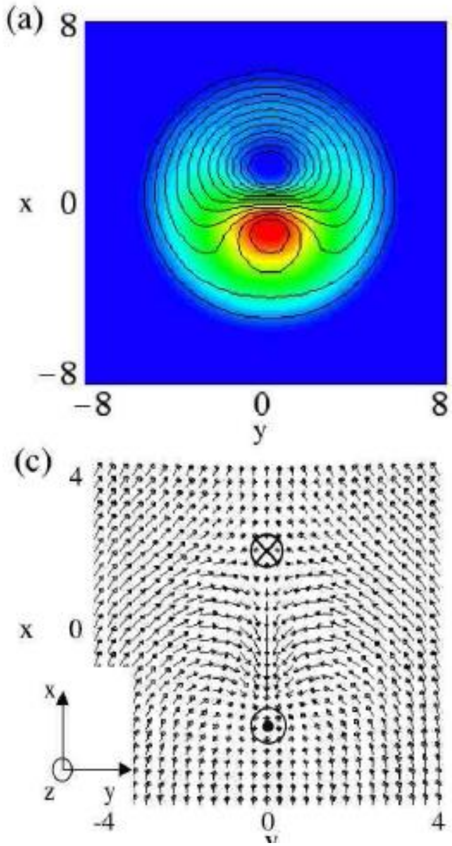


Defect is embedded into the regular stripe structure (black lines).
+/- are the alternating signs of the order parameter amplitude.
Termination points of a finite segment L (red color) of the zero line must be encircled by semi-vortices of the π rotation (blue circles) to resolve the signs conflict.

The microscopic modeling of the vortices splitting in a SC:

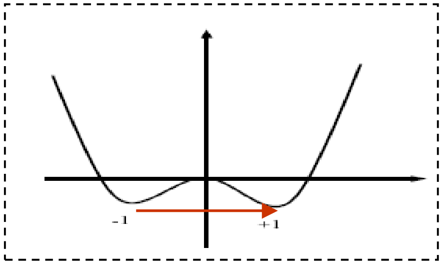
A numerical solution of discretized Bogolubov-De Gennes eqs. At presence of unpaired spins, the vortex created by rotation (magnetic field) splits into two semi-vortices.

Spatial Line Nodes and Fractional Vortex Pairs in the FFLO Vortex State of Superconductors
D. F. Agterberg, Z. Zheng, and S. Mukherjee 2008



Vortex molecules in coherently coupled two-component Bose-Einstein condensates
K. Kasamatsu, M.Tsubota, and M. Ueda 2004

Amplitude kinks in systems with complex order parameter : CDW, SC



Experimental puzzle and inspiration:

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

Obstacle: topological confinement :

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

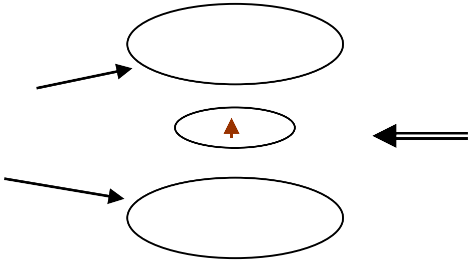
We need to activate other modes to cure the defect

RESOLUTION – combined symmetry $\mathbf{U_1/Z_2}$ of the order parameter **Aexp(i)**

Amplitude soliton (kink) **A ⇔-A**

together with ½-integer vortex of the phase **φ→φ+π,**

leaves invariant the order parameter



Half integer vortices: other examples in condensed matter.

Common basis:

multiplicative order parameter O=O1xO2 … factors possess degeneracies in different degrees of freedom.

Common obstacle:

weak perturbations reducing at least one of continuous symmetries to discrete one, like spin anisotropy in SDWs.

First proposal

(Volovik and Mineev 1976) A phase in superfluid He3

Never observed because of spin-orbital and dipole energies

$$O_{\alpha k} = A\boldsymbol{m}_{\alpha}\left(\boldsymbol{\Delta}'_{\boldsymbol{k}} + \boldsymbol{i}\boldsymbol{\Delta}''_{\boldsymbol{k}}\right)$$

$\boldsymbol{\Delta}' \times \boldsymbol{\Delta}'' = \boldsymbol{l}$ – orbital momentum of the Cooper pair

More recent hopes:

triplet superconductivity in $SrRuO_3$

Probably observed in nano-scale samples where the anisotropy energy had no volume to develop. J. Jang, et al, *Science* **331**, 186 (2011).

$$|\Delta|\hat{z}_\alpha \hat{k}_z e^{i\varphi} \qquad\qquad |\Delta|\hat{z}_\alpha (\hat{k}_x + i\hat{k}_y) e^{i\varphi}$$

Polariton condensate with the vector order parameter of condensed photons

Predicted by Rubo and soon clearly observed in Lagourdakis, et al, *Science* **326**, 974 (2009).

$$\mathbf{\Psi} = \mathbf{e}_\lambda |\psi| e^{i\varphi}$$

Conclusion

- Topologically nontrivial dynamics appears under applied fields or charge injection
- In SDW at low temperature, conventional dislocations loose their priority in favor of “himers” – the complex topological objects: a half-integer dislocation combined with a semi-vortex of the staggered magnetization .
- The combined topological objects are stabilized by lowering the Coulomb energy of dislocations especially important at low temperatures (Coulomb hardening)
- At presence of the magnetic anisotropy, the two combined objects are connected by the string – Neel domain wall.
- **Contrary to CDW the fundamental ratio NBN frequency to DC current is not the universal parameter**, changing from ½ near Tc to 1 at T<< Tc and being restorted to ½ in case of magnetic anisotropy.
- The numeric procedure needs to be stabilized for the nonanalytic eqs