Vortex-Vortex interactions in superconductors with nematic order

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Workshop on New Horizons in Quantum Correlated Materials

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departamento de física

EXACTAS UBA

PhD Thesis

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Vortices in a Ginzburg Landau Theory of Superconductors with Nematic Order

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Abstract

In this work we explore the interplay between superconductivity and nematicity in the framework of a Ginzburg Landau theory with a nematic order parameter coupled to the superconductor order parameter, often used in the description of superconductivity of Fe based materials. In particular, we focus on the study of the vortex-vortex interaction in order to determine the way nematicity affects its attractive or repulsive character. To do so, we use a dynamical method based on the solutions of the Time Dependent Ginzburg Landau equations in a bulk superconductor. An important contribution of our work is the implementation of a pseudo-spectral method to solve the dynamics, known to be highly efficient and of very high order in comparison to the usual finite differences/elements methods. The coupling between the superconductor and the (real) nematic order parameters is represented by two terms in the free energy: a biquadratic term and a coupling of the nematic order parameter to the covariant derivatives of the superconductor order parameter. Our results show that there is a competing effect: while the former independently of its competitive or cooperative character generates an attractive vortex-vortex interaction, the latter always generates a repulsive interaction.

- **General Introduction**
    - Electronic nematic phase in unconventional superconductors
    - Interplay between superconductivity and nematicity?

- **Model and numerical approach**
    - Ginzburg- Landau (GL) formalism in nematic superconductors
    - Dynamical approach based un TDGL equations solved by pseudo spectral methods
    - Results:
        - Superconducting vortices in nematic SC
        - Vortex-vortex interaction in nematic SC
    - Conclusions (1)

- **Outlook and perspective**

2006

FeSC

J|A|C|S
COMMUNICATIONS

Published on Web 07/15/2006

Iron-Based Layered Superconductor: LaOFeP

Yoichi Kamihara,† Hidenori Hiramatsu,† Masahiro Hirano,†,‡ Ryuto Kawamura,§ Hiroshi Yanagi,§ Toshio Kamiya,†,§ and Hideo Hosono*,†,‡

ERATO-SORST, JST, Frontier Collaborative Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan, Frontier Collaborative Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan, and Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-4, 4259 Nagatsuta, Yokohama 226-8503, Japan

Received May 15, 2006; E-mail: hosono@msl.titech.ac.jp

New type of non conventional superconductors

FeSC

Picnitides (Fe+ Group 15, like As)

Chalcogens (Fe+ Group 15, like Se)

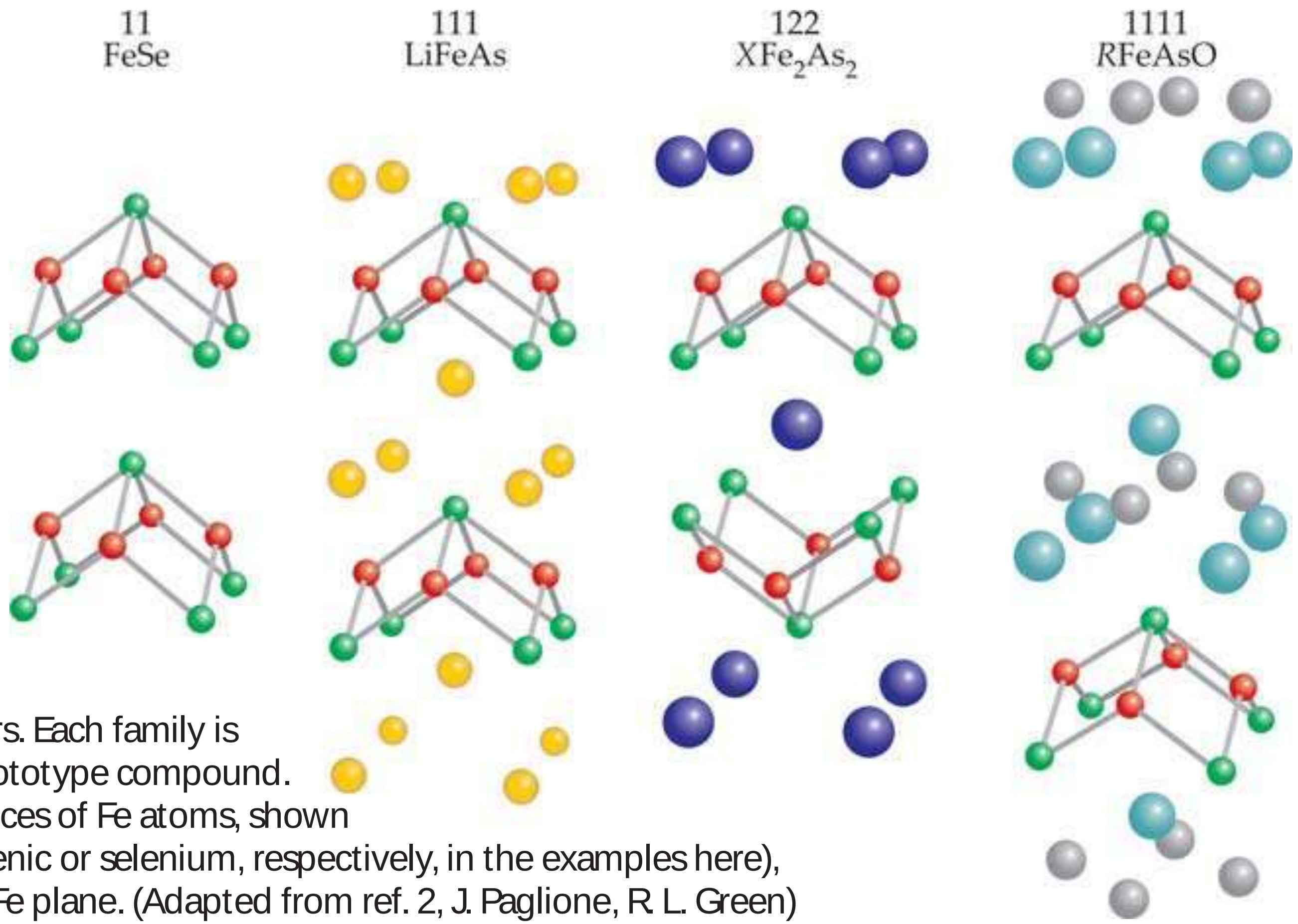

Figure 1. Crystallographic structures of various families of iron-based superconductors. Each family is labeled according to the stoichiometry of its prototype compound. Common to all systems is the set of square lattices of Fe atoms, shown in red, with pnictogen or chalcogen atoms (arsenic or selenium, respectively, in the examples here), shown in green, located above and below the Fe plane. (Adapted from ref. 2, J. Paglione, R. L. Green)

Microscopic Theory for Cuprates and FeSC not known yet

BUT

Indications that NEMATIC PHASES might play a fundamental rol

The topic

Electronic nematicity in unconventional superconductors

NATURE | VOL 393 | 11 JUNE 1998

Electronic liquid-crystal phases of a doped Mott insulator

S. A. Kivelson*, **E. Fradkin**† **& V. J. Emery**‡

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REVIEWS OF MODERN PHYSICS, VOLUME 87, APRIL–JUNE 2015

Colloquium: Theory of intertwined orders in high temperature superconductors

Eduardo Fradkin

Department of Physics & Institute for Condensed Matter Theory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801-3080, USA

Steven A. Kivelson

Department of Physics, Stanford University, Stanford, California 94305-4060, USA

John M. Tranquada

Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973-5000, USA

Annu. Rev. Condens. Matter Phys. 2010. 1:153–78

Nematic Fermi Fluids in Condensed Matter Physics

Eduardo Fradkin

Steven A. Kivelson

Michael J. Lawler

James P. Eisenstein

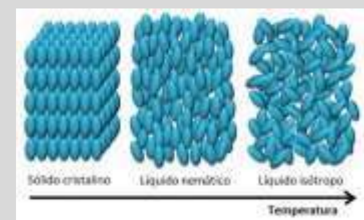
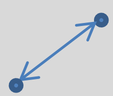
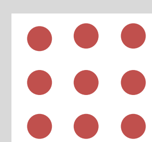
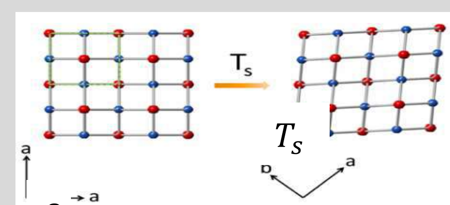
Andrew P. Mackenzie

Initially a theoretical proposal

The topic

Electronic nematicity in unconventional superconductors

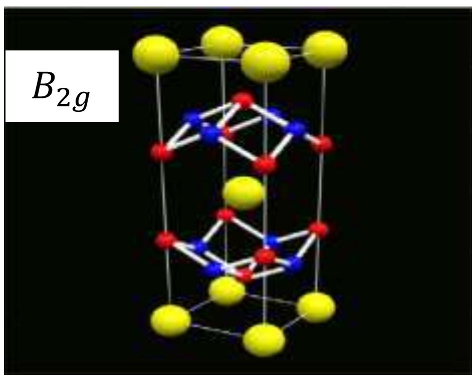
Electronic nematic phase

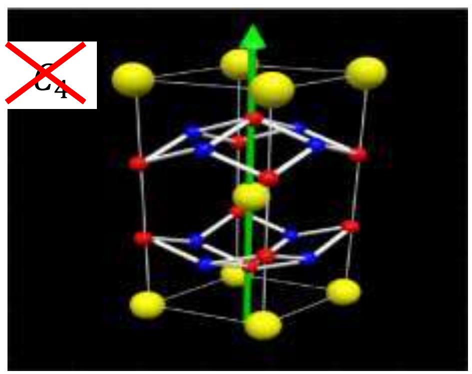
Nematic phase	Constituent elements	Environment	Broken Symmetry
Traditional: liquid crystals	Orientable molecules 	Free space	Continuous rotational symmetry 
Electronic	Strongly correlated electrons 	Ion Lattice 	Discrete rotational symmetry 

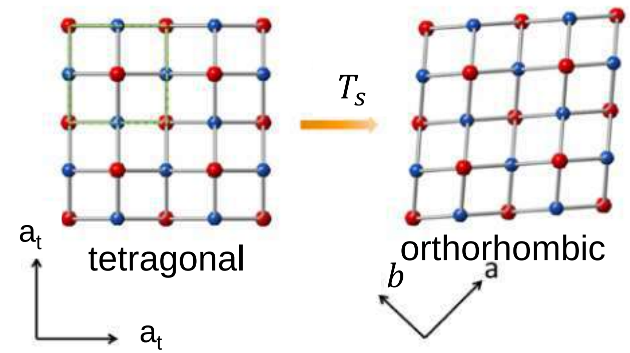
Electronic nematicity in unconventional superconductors

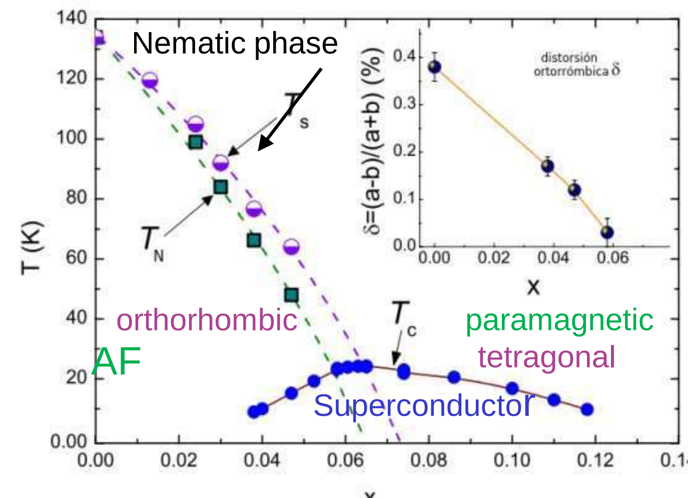
A spontaneous symmetry breaking in both structural and electronic properties below a critical temperature T_s.

Example : $\mathbf{Ba(Fe_{1-x}\,Co_x)_2As_2}$ (122)









R. Prozorov et. al., *Phys. Rev. Lett.* **80**, 174517 (2009)

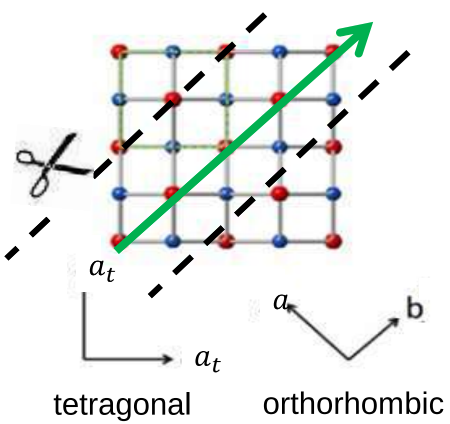
There is vast evidence that these transition is driven by electronic properties, giving rise to true **nematic phase transition**.

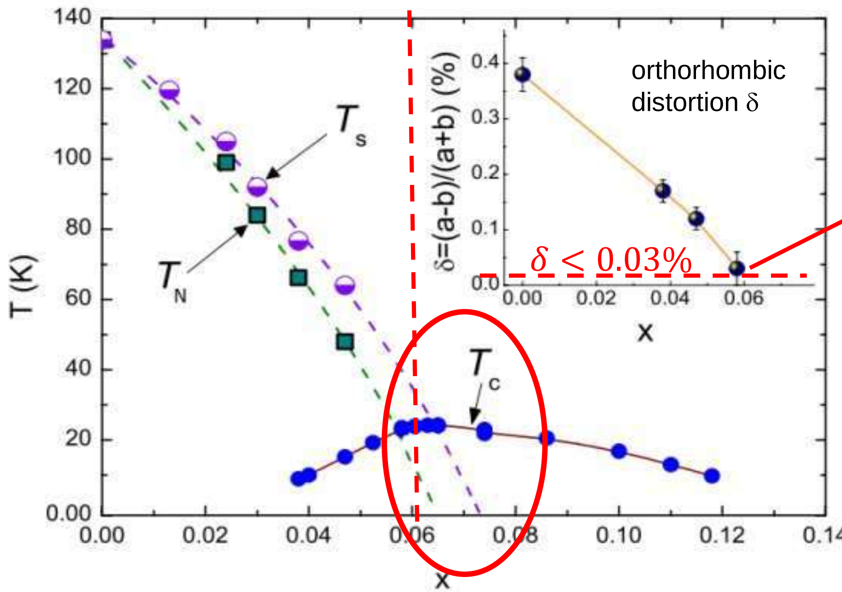
Experiments

Samples

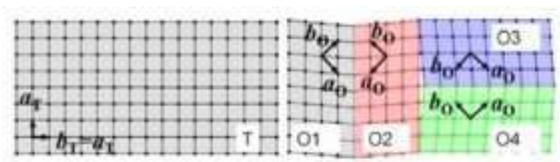
$Ba(Fe_{1-x}Co_x)_2As_2$ single crystals grown in P. C. Canfield's group (Ames Lab). Co dopping $x = 0.062$, near optimal.

Superconducting transition is undergone under nematic order, without long range magnetic order.





At $T < T_s$: Dense array of TBs with very subtle orthorhombic distortion.



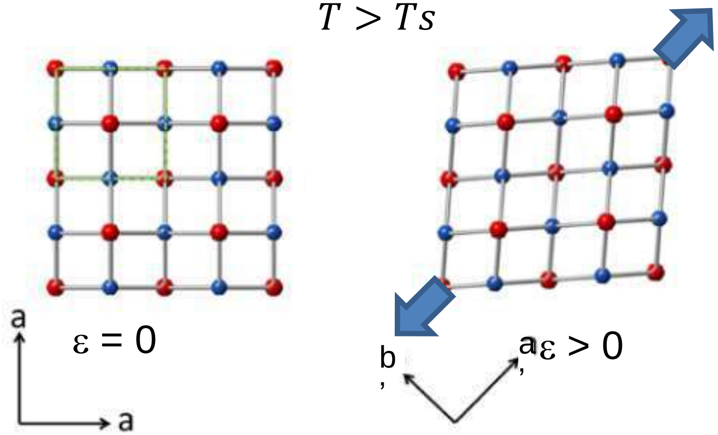
$T > T_S$ $T < T_S$

Samples cut along (110) tetragonal direction, (100) in orthorhombic axis.

Fase nemática electrónica

Evidence of nematicity in the metallic phase

tetragonal
$T > Ts$



If no external stress is present:

Tetragonal phase: $\eta \propto \frac{\rho_{a'} - \rho_{b'}}{\rho_{a'} + \rho_{b'}} = 0$

When a stress in applied .

" B_{2g} " (compress or pull a') $\varepsilon = \frac{\Delta L}{L}$:

$$\eta \propto \frac{\rho_{a'} - \rho_{b'}}{\rho_{a'} + \rho_{b'}}(\varepsilon) = \left(\frac{\Delta\rho}{\rho}\right)_{B_{2g}} = m^{B_{2g}}_{B_{2g}} \varepsilon_{B_{2g}} = m\varepsilon$$

Resistive anisotropy

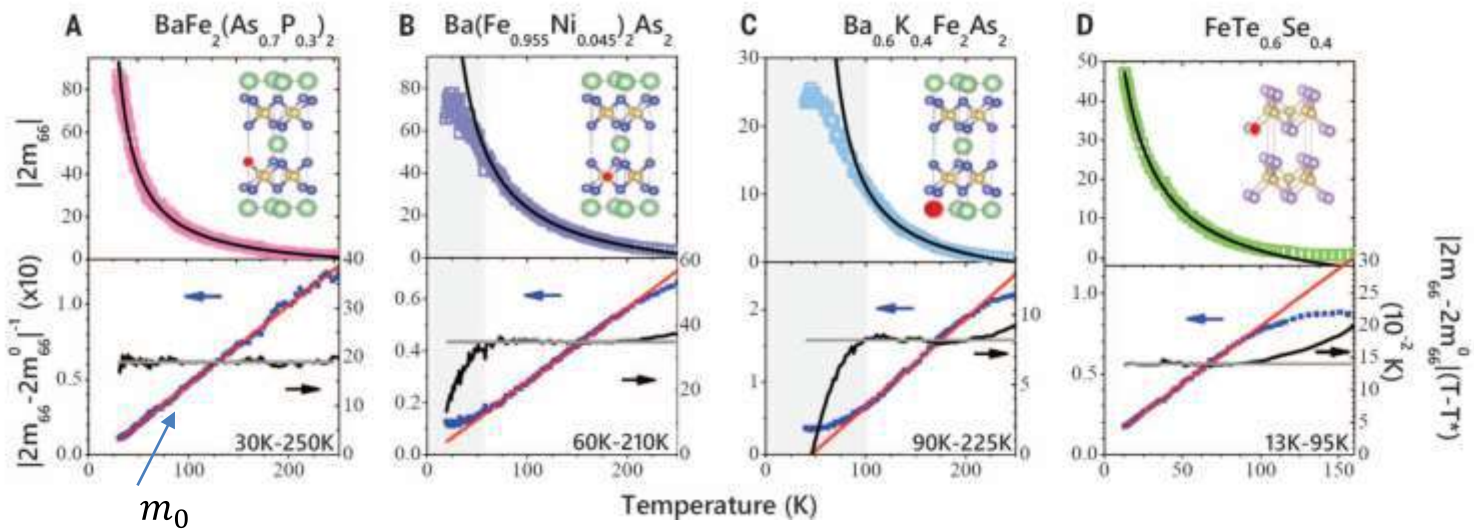
elasto-resistivity

simplifying

$$\boxed{\frac{\partial \eta}{\partial \varepsilon} \propto \frac{\partial(\Delta\rho/\rho)}{\partial \varepsilon} = m}$$

Nematic susceptibility

Evidence of nematic transition



$$m_{66} = \frac{m_0}{T - T^*}$$

H-H Kuo et al. *Science* **352**.6288 (2016)

Nematic susceptibility m_{66} , and Curie law

PHYSICAL REVIEW B **99**, 064515 (2019)

Nematicity in the superconducting mixed state of strain detwinned underdoped $Ba(Fe_{1-x}Co_x)_2As_2$

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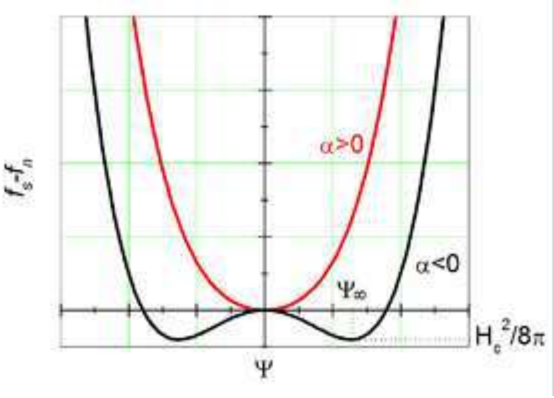
(Received 20 December 2018; revised manuscript received 11 February 2019; published 28 February 2019)

Evidence of nematic effects in the mixed superconducting phase of slightly underdoped $Ba(Fe_{1-x}Co_x)_2As_2$ is reported. We have found strong in-plane resistivity anisotropy for crystals in different strain conditions. For these compositions, there is no magnetic long-range order, so the description may be ascribed to the interplay between the superconducting and nematic order parameters. A piezoelectric-based apparatus is used to apply tensile or compressive strain to tune nematic domain orientation in order to examine intrinsic nematicity. Measurements are done under a rotating magnetic field, and the analysis of the angular dependence of physical quantities identifies the cases in which the sample is *detwinned*. Furthermore, the angular dependence of the data allows us to evaluate the effects of nematicity on the in-plane superconductor stiffness. Our results show that although nematicity contributes in a decisive way to the conduction properties, its contributions to the anisotropy properties of the stiffness of the superconducting order parameter is not as significant in these samples.

Ginzburg Landau Theories

Superconductivity 1911

Ginzburg – Landau (1950)



Modelo Bardeen – Cooper – Schrieffer (BCS) (1957)

Nematic-superconducting coupling

Interplay between nematicity and superconductivity

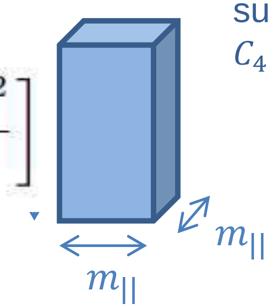
Ginzburg Landau (GL) approach

$\mathcal{F}_{sc}$

$$F_s = \int dV \left[\alpha_{GL}|\psi|^2 + \frac{\beta_{GL}}{2}|\psi|^4 + \frac{\hbar^2}{2m}|\boldsymbol{D}\psi|^2 + \frac{(\nabla \times \boldsymbol{A})^2}{8\pi} \right]$$

$$\frac{\partial}{\partial x_\mu} + \frac{i2e}{hc}A_\mu$$

quasi- tetragonal superconductor: C_4 symmetry .



$$\gamma = \sqrt{\frac{m_\perp}{m_{||}}}$$

Superconducting . anisotropy

$$a = a_0(T - T^*)$$

Ginzburg Landau parameter

$$\xi_\mu^2 = \frac{\hbar^2}{2m_\mu|\alpha|}$$

$$\lambda_L^2 = \frac{m_\mu c^2 \beta}{4\pi e^2 \alpha}$$

$$\kappa = \frac{\lambda}{\xi}$$

...

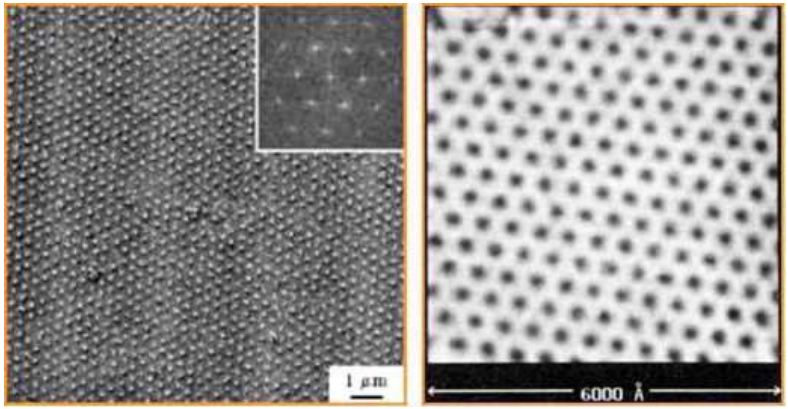
Superconductor Coherence length

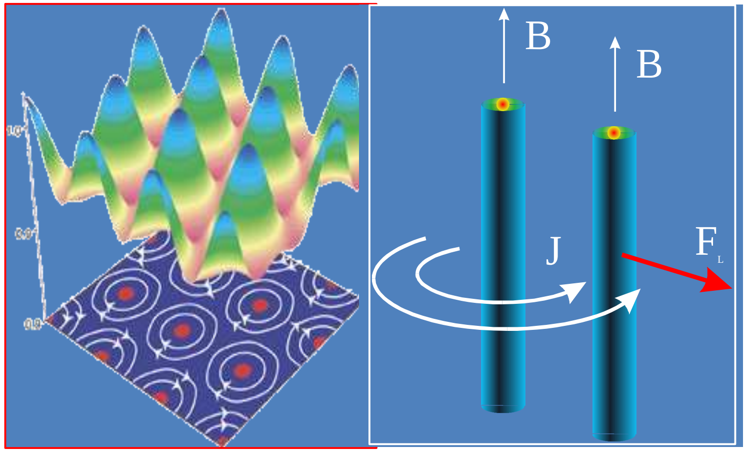
London Length

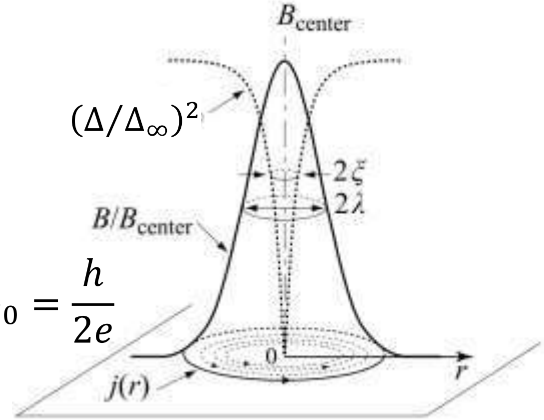
Ginzburg Landau parameter

Limit between type I and type II superconductors

$$\kappa > \kappa_c = \frac{\lambda_L}{\xi} = \frac{1}{\sqrt{2}}$$



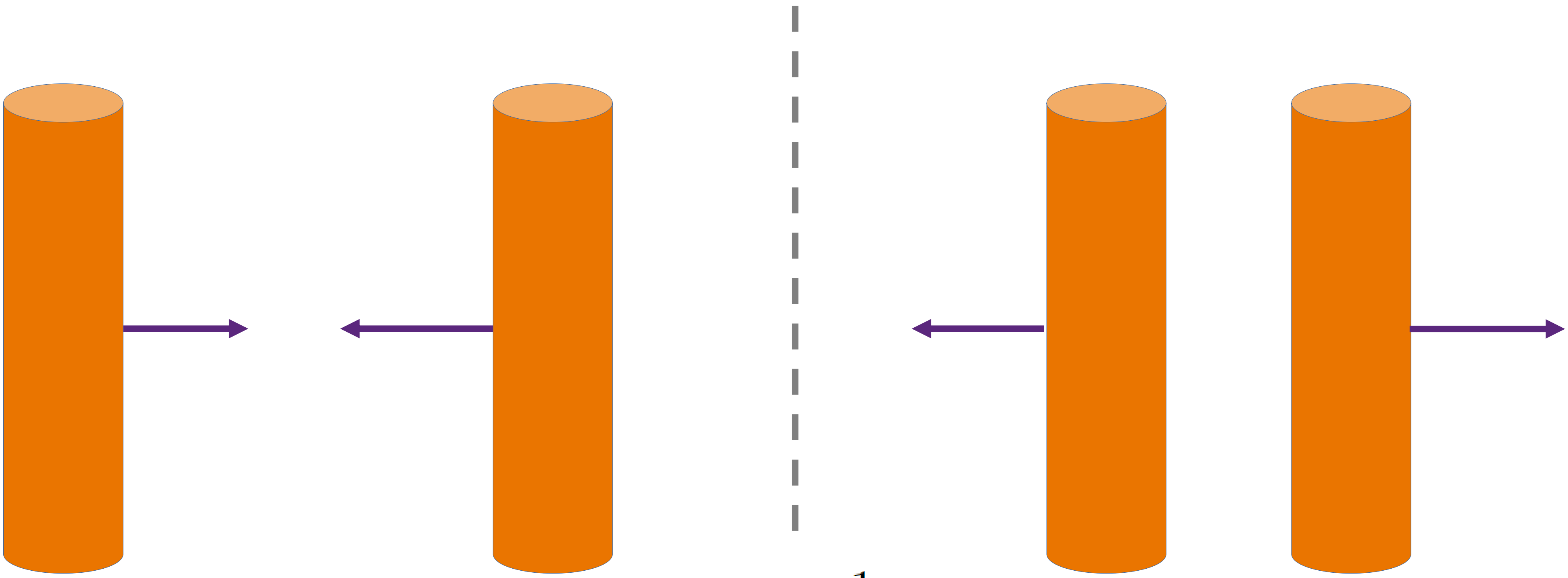




$$\phi_0 = \frac{h}{2e}$$

The Nobel Prize in Physics 2003

Vortex Vortex Interaction in the standard GL model



$\kappa < \kappa_c$

Attraction

$$\kappa_c = \frac{1}{\sqrt{2}}$$

Non Interacting

$\kappa > \kappa_c$

Repulsion

Ginzburg – Landau nematic

$$F_s = \int dV \left[\alpha_{GL}|\psi|^2 + \frac{\beta_{GL}}{2}|\psi|^4 + \frac{\hbar^2}{2m}|\boldsymbol{\mathcal{D}}\psi|^2 + \frac{(\nabla \times \boldsymbol{A})^2}{8\pi} \right]$$

Ising type order parameter

$$F_N = \int_V dV \left[\underbrace{\gamma_2 (\nabla \eta)^2 + \gamma_3 \eta^2 + \frac{\gamma_4}{2}\eta^4}_{\text{Pure nematic energy}} + \underbrace{\frac{\hbar}{2m}\lambda_1 \eta (|\mathcal{D}_x \psi|^2 - |\mathcal{D}_y \psi|^2)}_{\text{Truly nematic coupling}} + \underbrace{\lambda_2 \eta^2 \psi^2}_{\text{Bi quadratic coupling}} \right]$$

Pure nematic energy

Truly nematic coupling

Bi quadratic coupling

Nematic symmetry is broken if

$$\gamma_3 < 0$$

How do we describe time dependent phenomena?

- Normally a Free Energy is thermodynamical concept suited to describe equilibrium

- A standard procedure to describe out of equilibrium evolution Is via dissipative dynamics.

$$\gamma \frac{dx}{dt} = -\frac{\delta H}{\delta x}$$

Whre x is a dynamical variable and γ Is a dissipative constant

Interplay between nematicity and superconductivity

Solving the Time Dependent GL Dynamics: an alternative approach

$$F_s = \int dV \left[\alpha_{GL}|\psi|^2 + \frac{\beta_{GL}}{2}|\psi|^4 + \frac{\hbar^2}{2m}|\boldsymbol{\mathcal{D}}\psi|^2 + \frac{(\nabla\times\mathbf{A})^2}{8\pi} \right]$$

Time Dependent GL Dynamics
TDGL
Schmid ´60

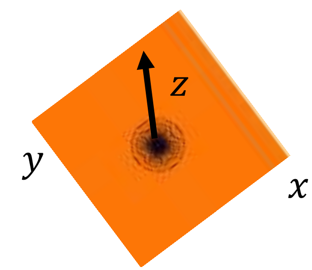
$$\begin{cases} \dfrac{\hbar^2}{2m\mathcal{V}_s}\partial_t\psi = -\dfrac{\delta\mathcal{F}}{\delta\psi^*} \\[2ex] \dfrac{\sigma}{c^2}\partial_t\boldsymbol{A} = -\dfrac{\delta\mathcal{F}}{\delta\boldsymbol{A}} \end{cases}$$

$\mathcal{V}_s$
diffusion constants

σ normal conductivity

Non-Linear differential equations ussually solved using finite Difference methods (but we will do in a different way)

$\psi\,(x,y,t)$
$B_z(x,y,t)$



Interplay between nematicity and superconductivity
Solving the Time Dependent GL Dynamics: an alternative approach

A theoretical problem:
- We are able to control the total magnetic flux ϕ
- Fixed controlled temperature T

Stable configurations minimize
$$\mathcal{F} = \mathcal{F}_{sc} + \mathcal{F}_{nem} + \mathcal{F}_{int}^{2} + \mathcal{F}_{int}^{1}$$

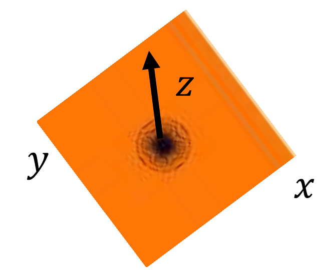
Time Dependent GL Dynamics
The simplest problem: Bulk infinite clean superconductor

$$\left\{ \begin{aligned} \frac{\hbar^2}{2m\mathcal{V}_s}\partial_t \psi &= -\frac{\delta\mathcal{F}}{\delta\psi^*} \\ \frac{\hbar^2}{2m\mathcal{V}_n}\partial_t \eta &= -\frac{\delta\mathcal{F}}{\delta\eta} \\ \frac{\sigma}{c^2}\partial_t \boldsymbol{A} &= -\frac{\delta\mathcal{F}}{\delta\boldsymbol{A}} \end{aligned} \right.$$

$\mathcal{V}_s$ and $\mathcal{V}_n$ diffusion constants

σ normal conductivity

$\psi\,(x, y, t)$
$\eta(x, y, t)$
$B_z(x, y, t)$



Numerical solution by using pseudo spectral methods (numerical code GHOST) developed to study quantum fluids .

P. D. Mininni et al. *Parallel Computing*, **37**(6):316 (2011)

https://github.com/pmininni/GHOST

GHOST

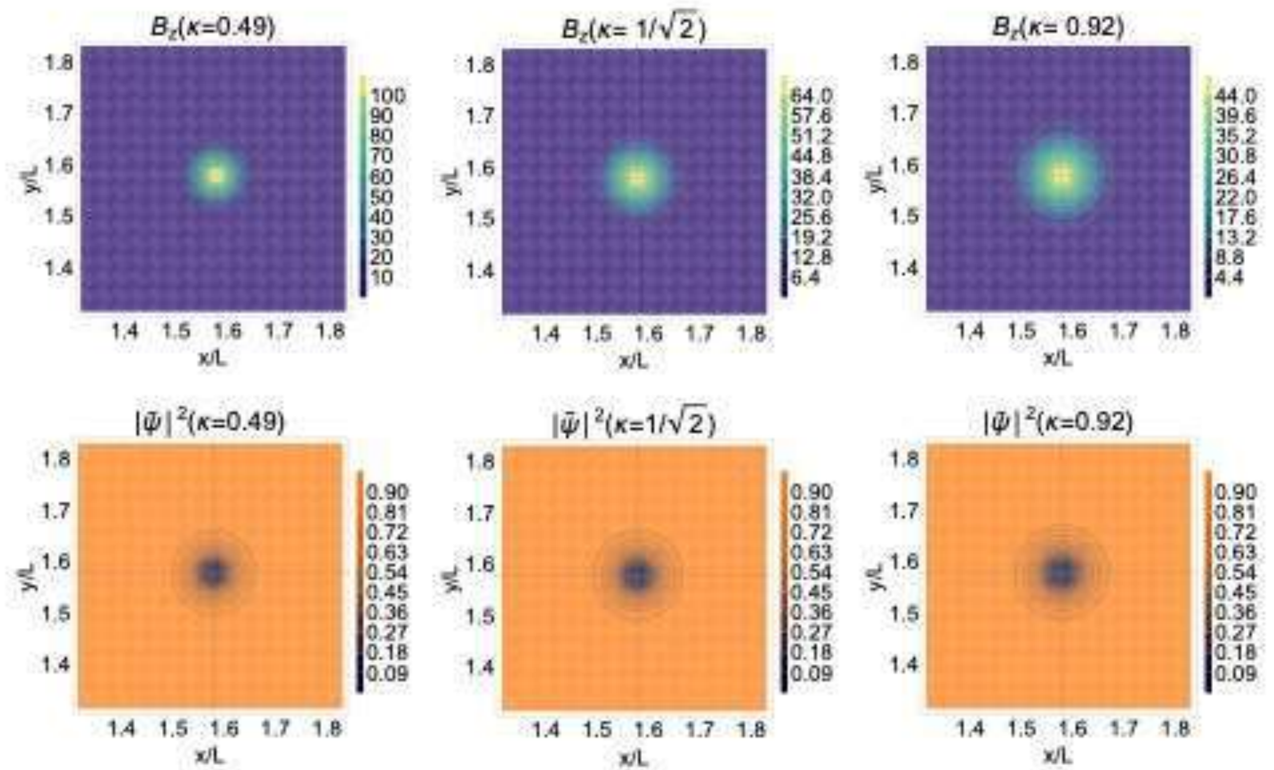
GHOST (the *Geophysical High-Order Suite for Turbulence*) is an accurate and highly scalable pseudospectral code that solves a variety of PDEs often encountered in studies of turbulent flows. It is developed in collaboration with Duane Rosenberg and with contributions from many users. The code uses a hybrid parallelization method combining MPI and OpenMP (GHOST also has support for GPUs using CUDA). This allows the code to run efficiently in laptops and small clusters, as well as to scale up to 100,000 CPU cores in production runs in supercomputers. It can also combine CPU and GPU computations when needed. This hybrid parallelization method was recognized by two awards: an NCAR/CISL award to Pablo Mininni and Duane Rosenberg, and the best paper award (technology track) at the TeraGrid 2010 conference.

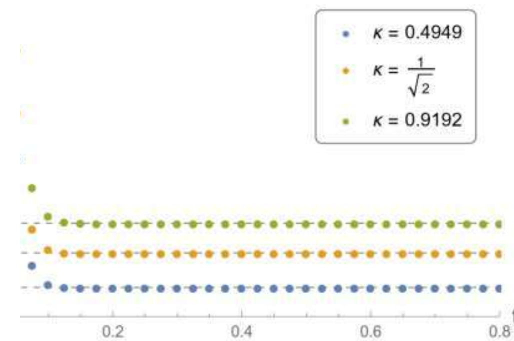
GHOST can solve PDEs in periodic domains in two and three dimensions, to tackle many problems including:

Checking the numerical methods with known results

One vortex solution for different κ

Magnetic fied





Superconducting order parameter

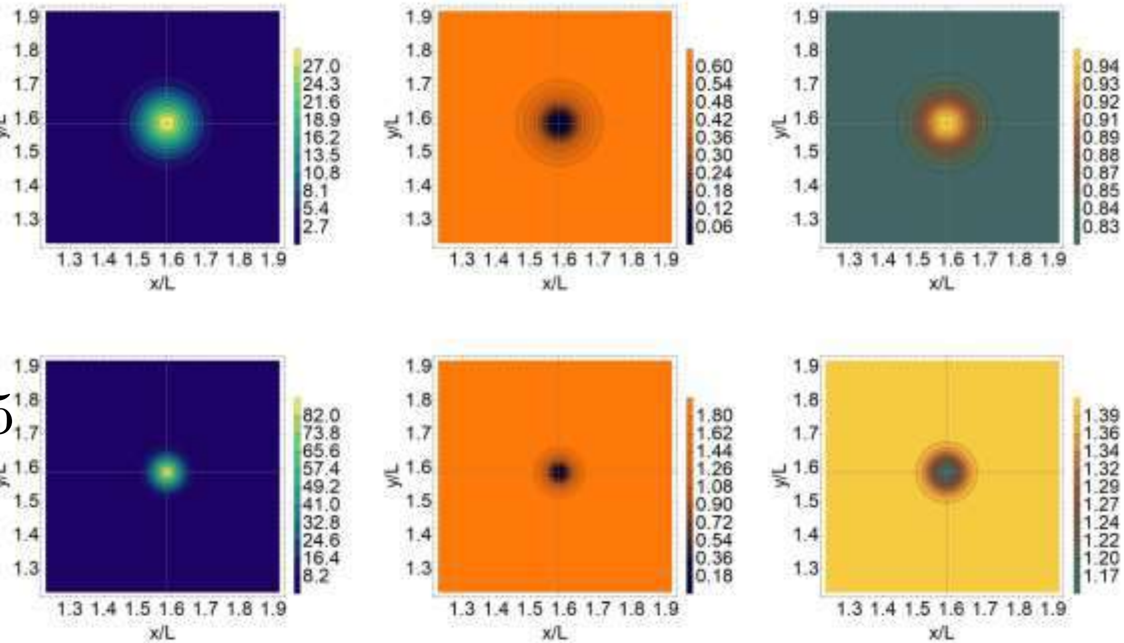
Effects of biquadratic coupling

one vortex

$$\mathcal{F}^2_{int} = \lambda_2 \int d^3\mathbf{r}\ \eta^2|\Delta|^2$$

$\hat{\lambda}_2 = 0.5$

$\hat{\lambda}_2 = -0.5$



Magnetic SC Nematic

Nematic order increases in vortex core
competition

Nematic order decreases in vortex core
cooperation

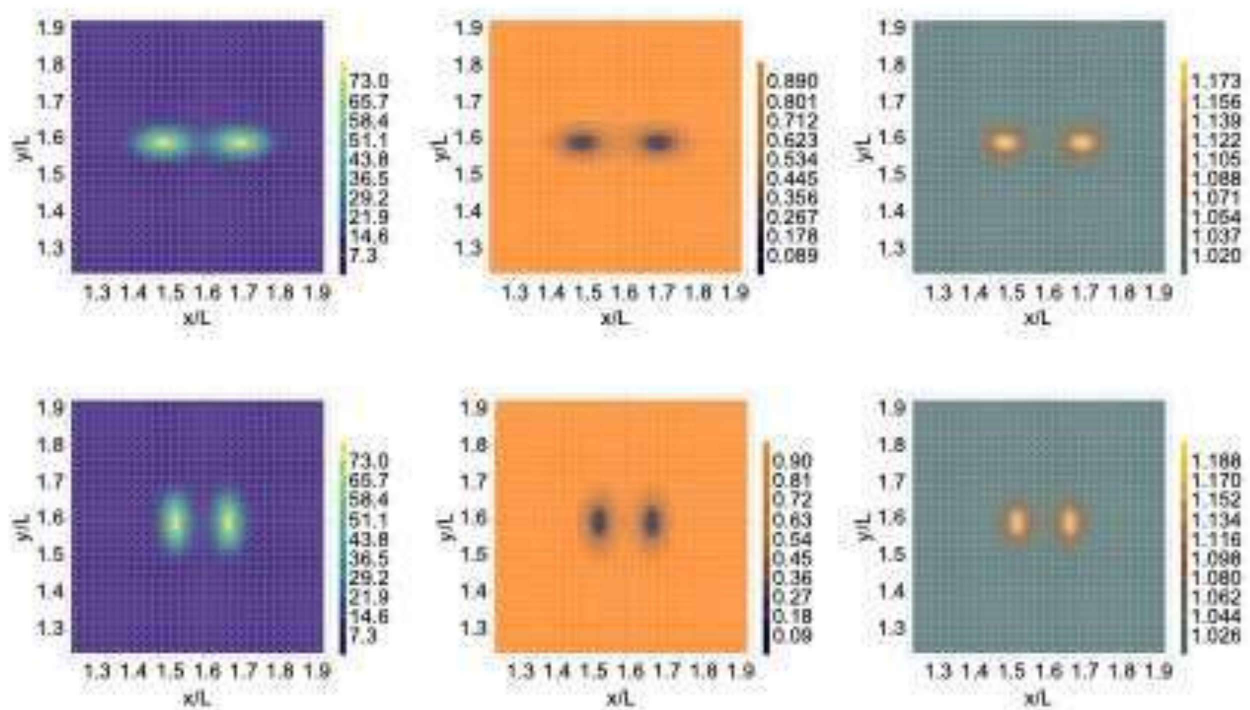
Effects of the gardient coupling

one vortex

$$\mathcal{F}^{1}_{int} = \frac{\lambda_1}{2}\int \mathrm{d}^3\mathbf{r}\,\eta\left\{|D_x\Delta|^2 - |D_y\Delta|^2\right\}$$

$\hat{\lambda}_1 = 0.5$

$\hat{\lambda}_1 = -0.5$



Elliptical vortices

“nematic coupling”

How does the presence of this couplings change the vortex-vortex interaction?

Self Dual Equations

In the standar GL theory, the attractive and repulsive character of the vortices, and the excistence of a critical value κ_c=1/$\sqrt{2}$ can be shown exactly using a trick due to Bogomol´nyi (1975).

This point has deep mathematical and physical consequences (Self Dual Equations, Topological Field Theories, Supersymmetry, BPS states).

At κ_c=1/$\sqrt{2}$, the energy is proportional to the vorticity, indicating vortices do not interact.

$$E(N) = N\,E(1) = N\Phi_1$$

Self Dual Equations for nematic order

Vortex-vortex interaction in Nematic Superconductors

1) SC coupled with a fixed nematic background
(**single nematic domain with** $\eta = \eta_0$)

$$\boxed{\kappa_c^2 = \frac{1}{2}\left[1 - \left(\frac{\lambda_1 \eta_0}{}\right)^2\right]}$$

Analytical solution for the self-dual point

A bilinear nematic $\lambda_1 \eta_0 \neq 0$ always favors type II SC
ATTRACTIVE INTERACTION

The biquadratic coupling λ_2 does not affect κ_c
(in the limit of constant nematicity)

2) General numerical solution with
SC-nematic coupling

$\kappa < \kappa_c$ $\kappa \sim \kappa_c$ $\kappa > \kappa_c$

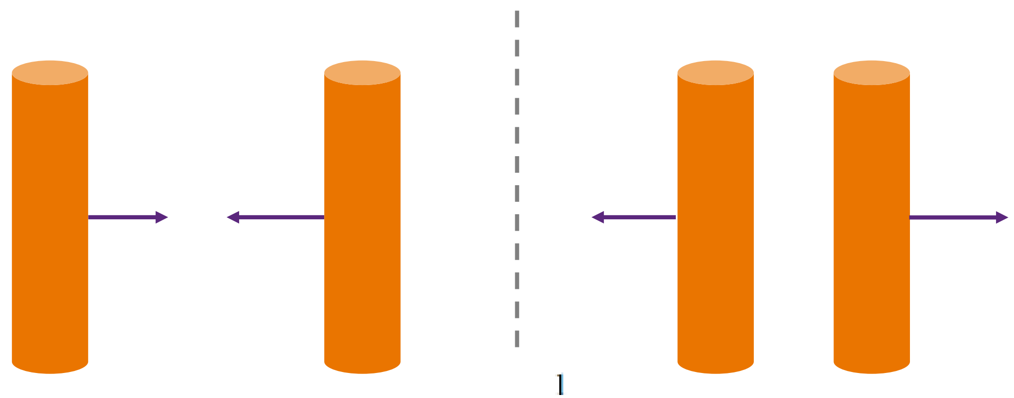
attraction repulsion

κ_c is obtained from the limit between
vortex- vortex attraction and repulsion
(non interacting vortices within our numerical resolution)

E. B. Bogomolny. *Sov. J. Nucl. Phys*, 24:449, 1976
R. Severino, P. Mininni, E. Fradkin, V.Bekeris, G.Pasquini, and G. S. Lozano , preprint (2022)
...

Self Dual Equations for nematic order

Vortex-vortex interaction in Nematic Superconductors



2) General numerical solution with SC-nematic coupling

$\kappa < \kappa_c$ attraction

$\kappa \sim \kappa_c$

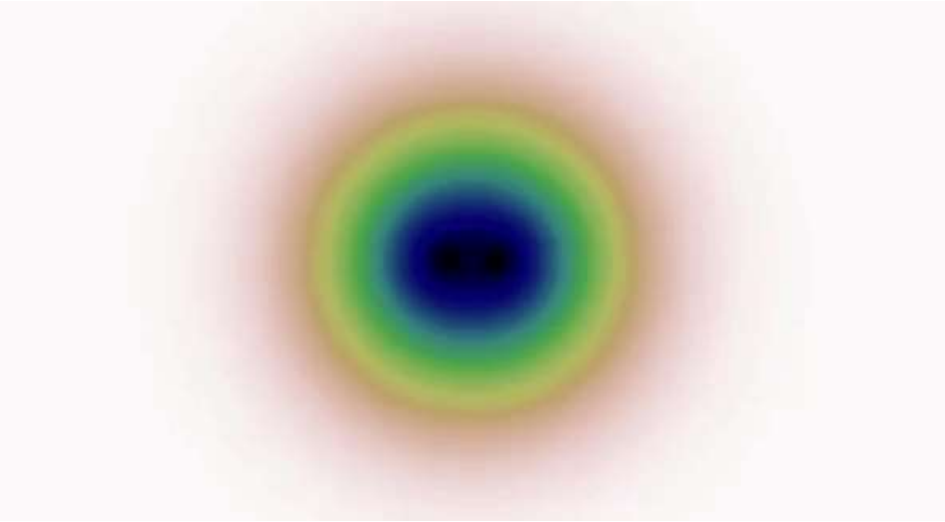
$\kappa > \kappa_c$ repulsion

κ_c is obtained from the limit between vortex- vortex attraction and repulsion

…(non interacting vortices within our numerical resolution)

NUMERICS

We use pseudo spectral methods to solve TDGL. We use **Geophysical High-Order Suite for Turbulence (GHOST)**



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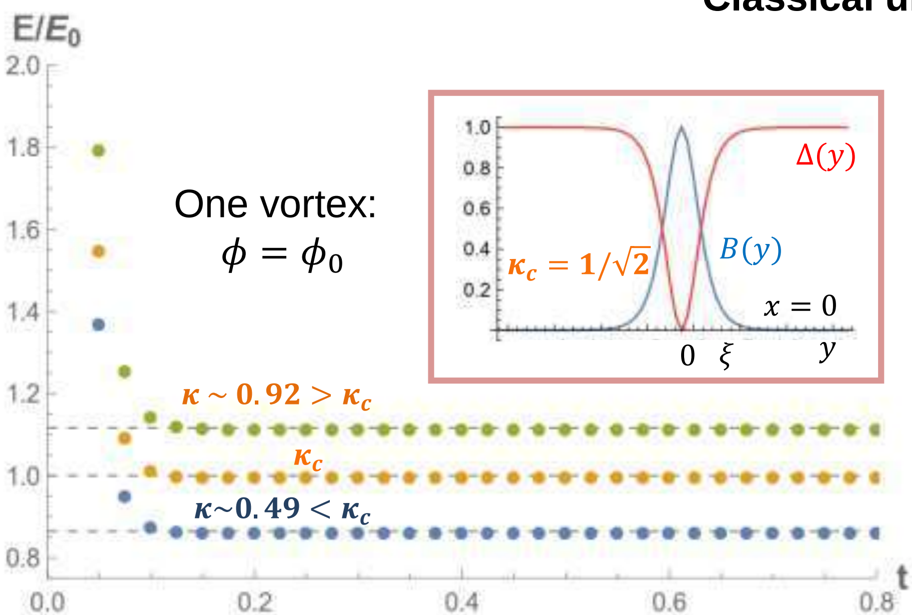
Resulsive interaction (no nematicity)

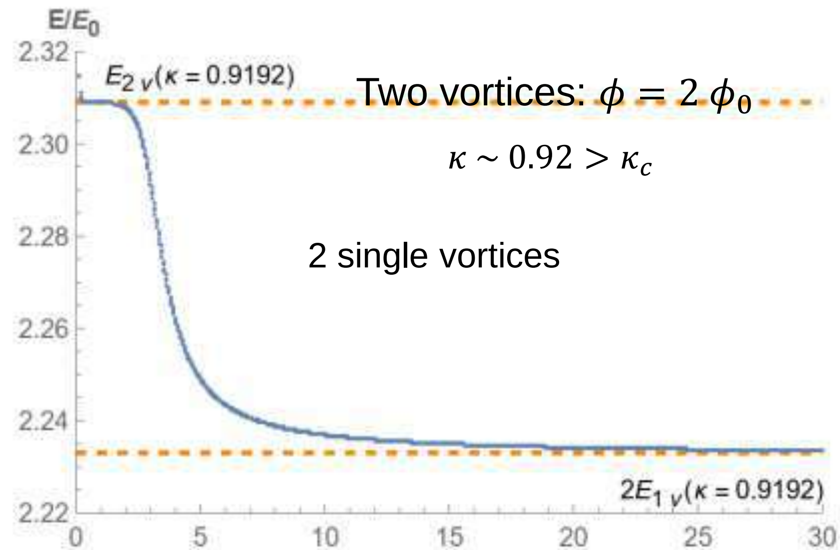
Interplay between nematicity and superconductivity

Solving the dynamics with pseudo spectral methods (an alternative approach).

Classical uncoupled SC



1 giant vortex



Fast and accurate convergence
No numerical dispersion

Repulsive vortex-vortex interaction for $\kappa > \kappa_c = 1/\sqrt{2}$
Attractive vortex-vortex interaction for $\kappa < \kappa_c = 1/\sqrt{2}$

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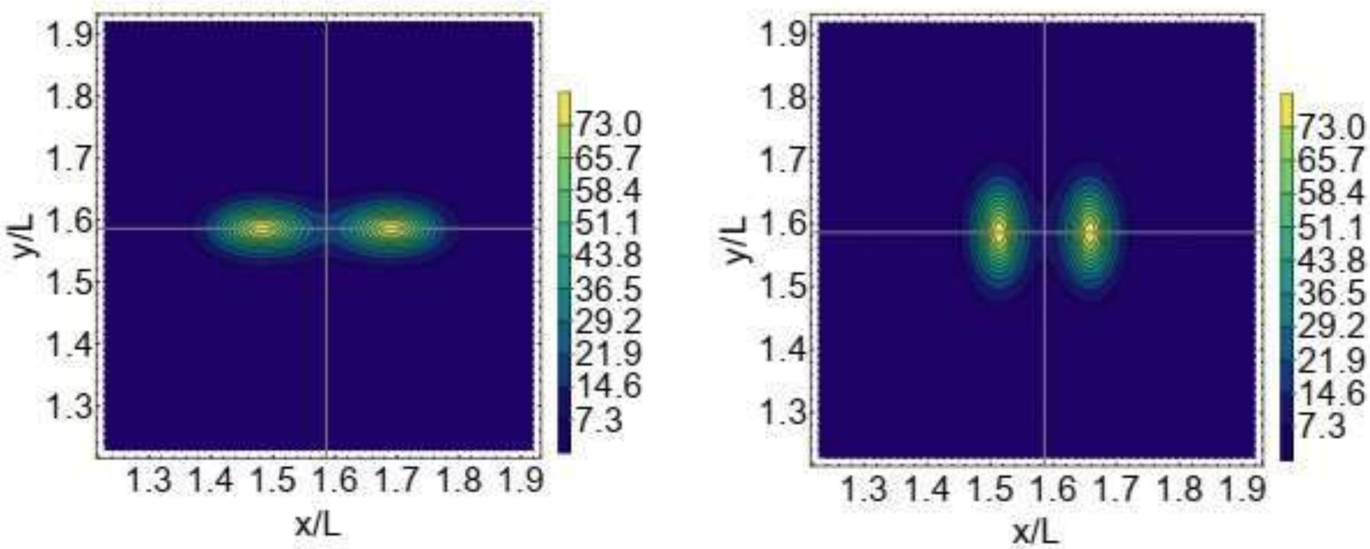
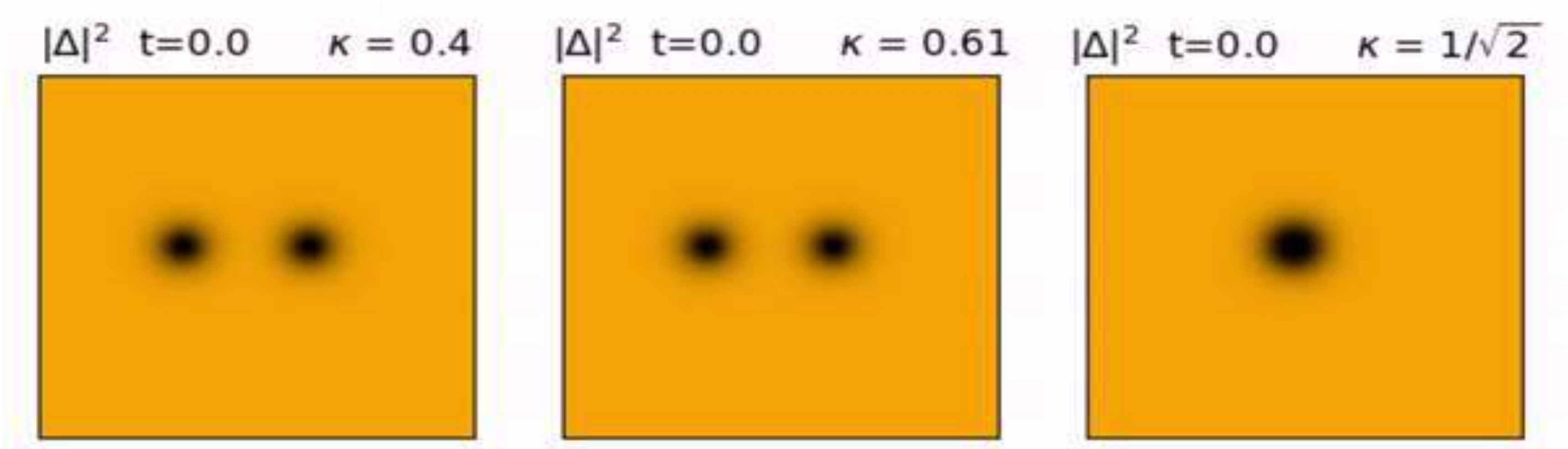
R. Severino, P. Mininni, E. Fradkin, V.Bekeris, G.Pasquini, and G. S. Lozano , preprint (2022)

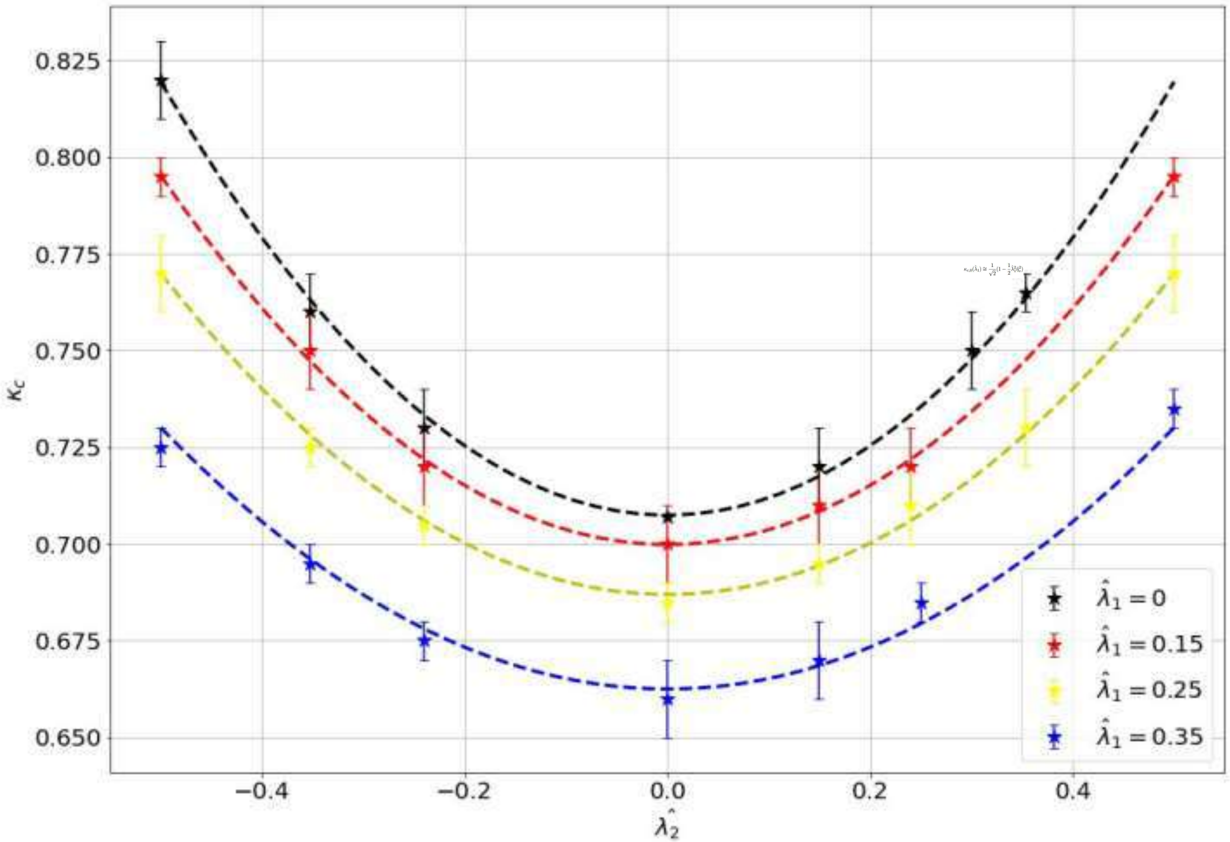
Elliptical Vortices. Vortex-Vortex interaction



We use dynamics to determine the critical value



We determine how nematiciy affects the value of κ_c



$$\kappa_c = \kappa_{c,0}(\hat{\lambda}_1) + a(\hat{\lambda}_1)\hat{\lambda}_2^2.$$

$$\kappa_{c,0}(\hat{\lambda}_1) \cong \frac{1}{\sqrt{2}}(1 - \frac{1}{2}\hat{\lambda}_1^2\tilde{\eta}_v^2)$$

Gradiente coupling-> Repulsion

Biquadratic coupling ->Attraction

Energy (and force) as function of separation

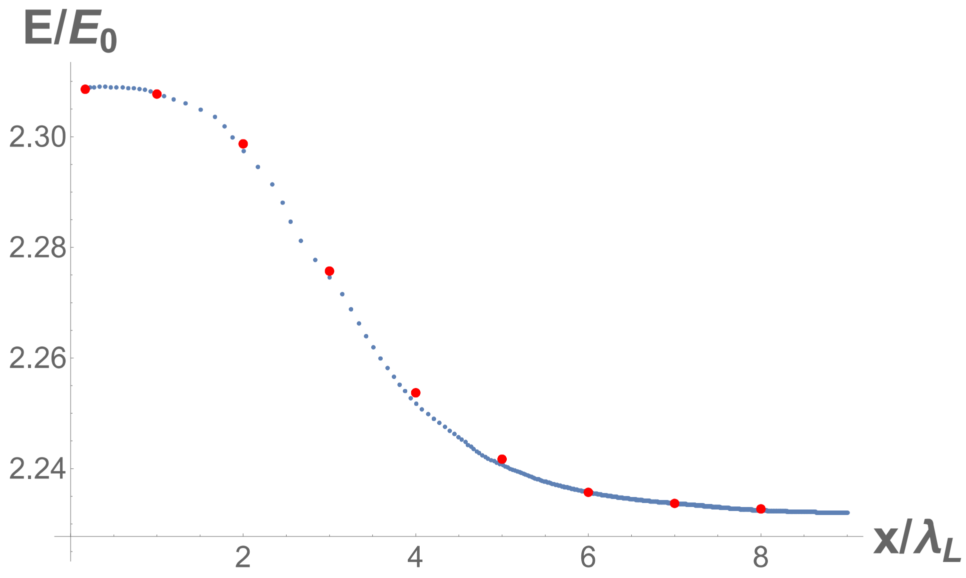
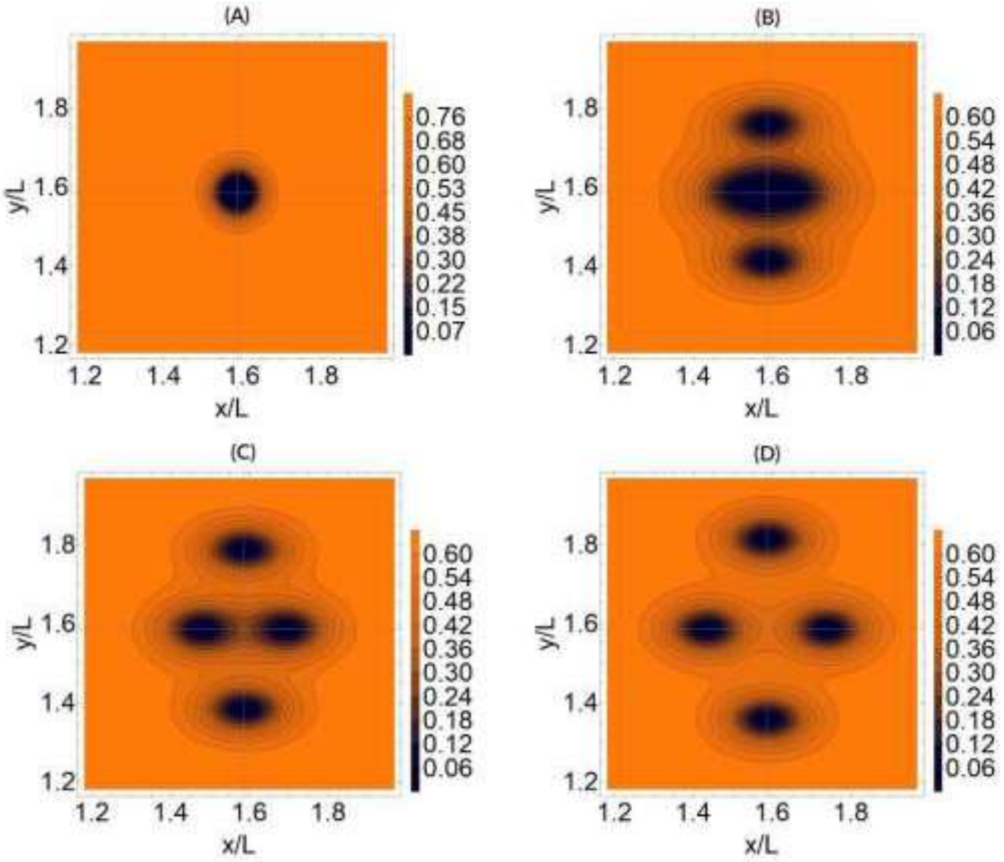


FIG. 12. Energy as a function of intervortex distance for $\kappa = 0.92$. The red dots are values taken from Ref. [5].

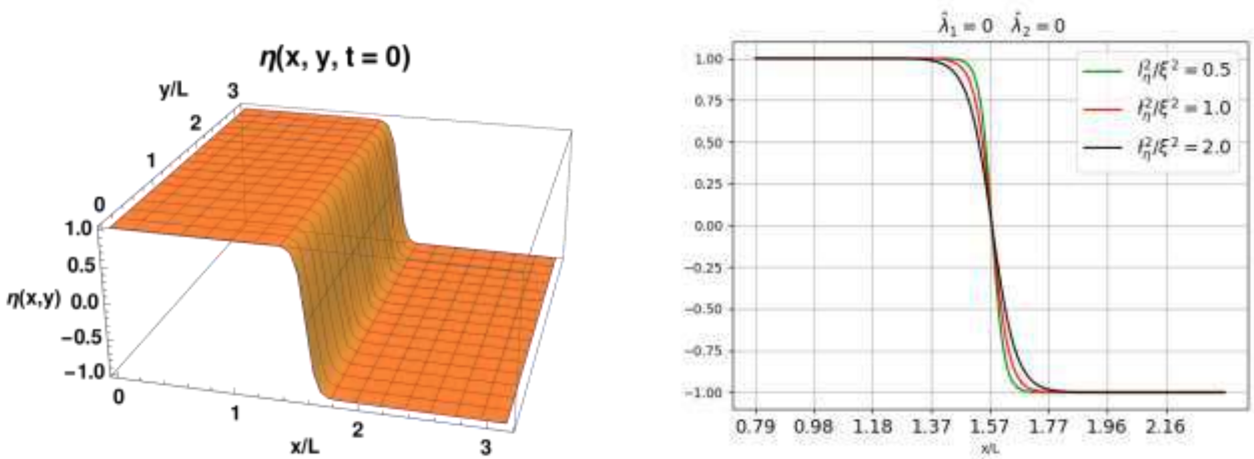
Playing with N-vortices



N=4

Whats is next?

Pining by nematic walls?



(a) (b)

FIG. 1. (a)Plot of the initial condition for the nematic order parameter simulating a domain wall on the *xy* plane (b) Profiles along the x axis for three diﬀerent domain walls, varying the nematic coherence length l_η. The coherence length is directly related to the width of the wall.

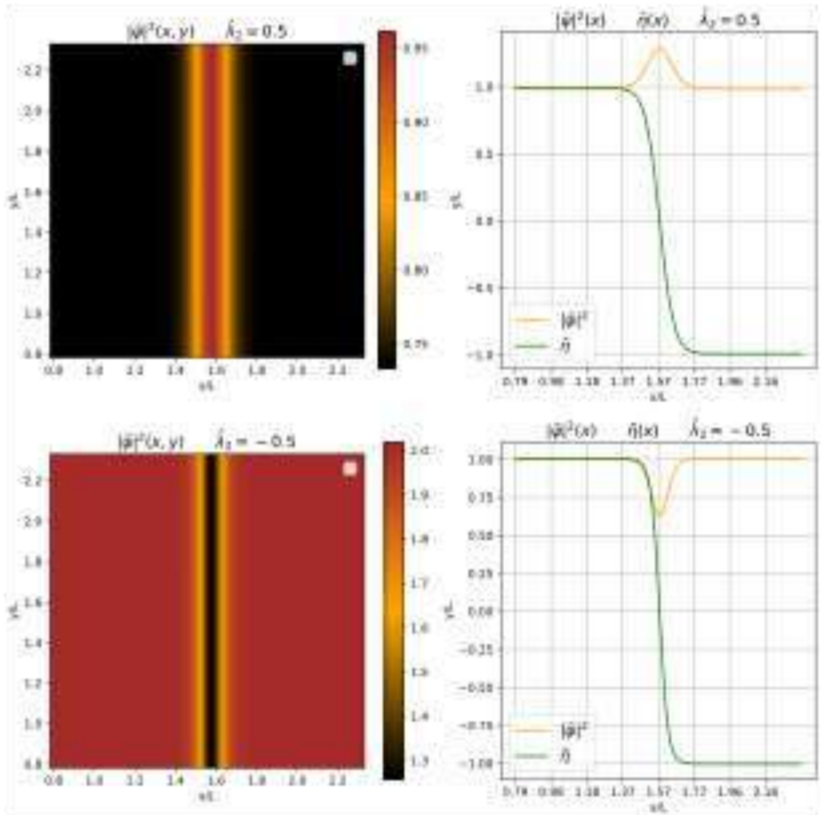


FIG. 2. Density plot of $|\tilde{\psi}|^2$ along with profiles for $|\tilde{\psi}|^2(x)$ and $\tilde{\eta}(x)$ on the line $(x, \pi/2)$ for positive (top row) and negative (bottom row) coupling parameter $\tilde{\lambda}_2$. Notice that the order parameter is enhanced or depressed on the domain wall based on the sign of the coupling parameter, as it happened on the vortices case.

Vortex pining by a domain wall

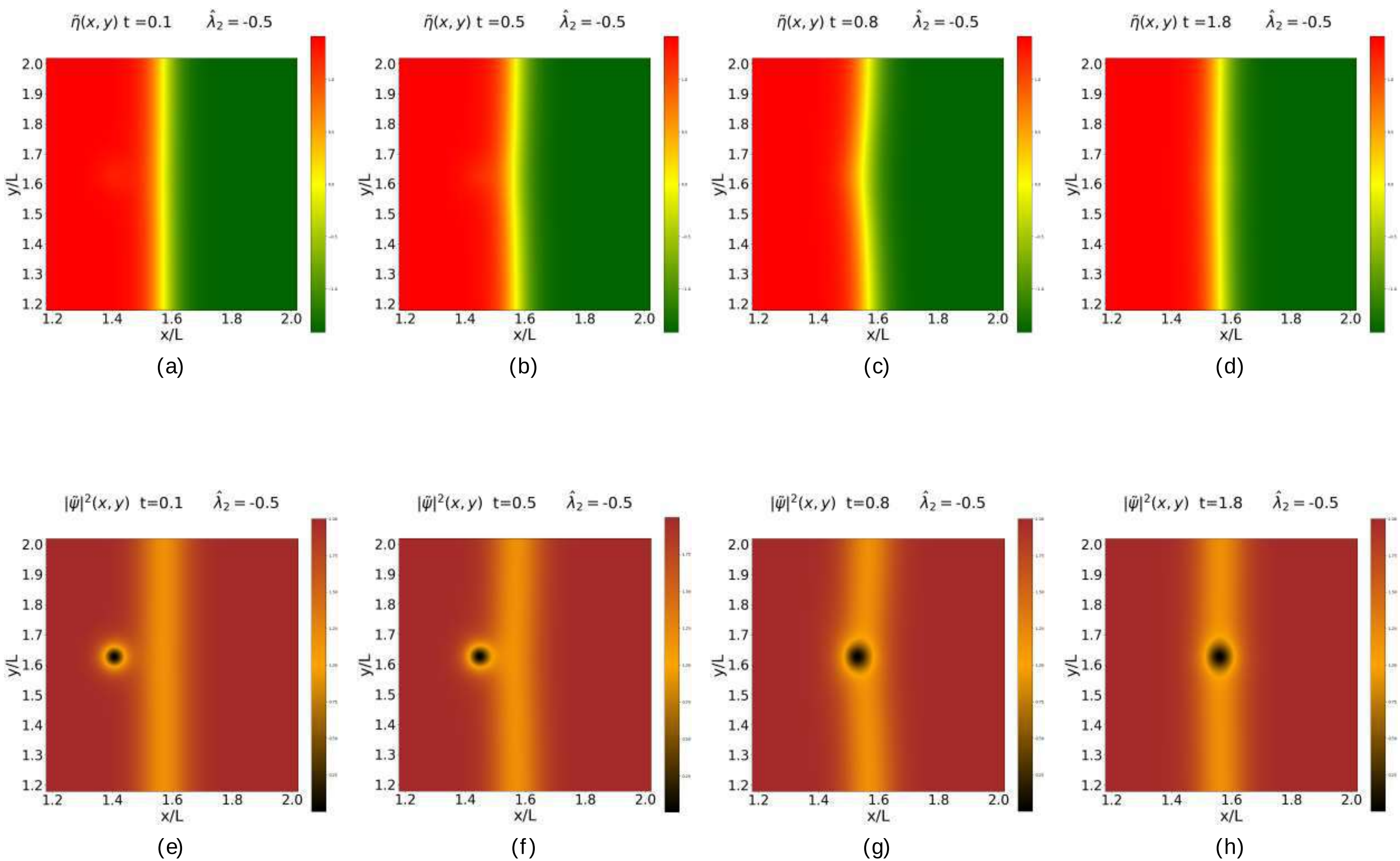
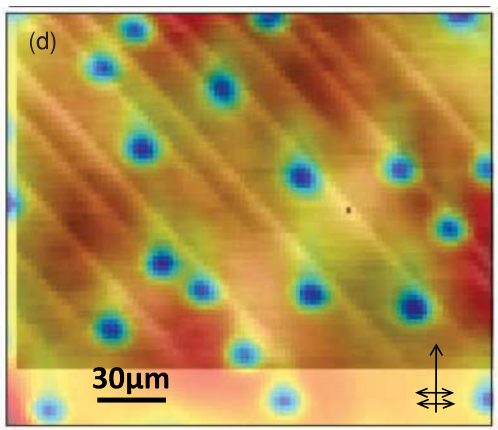
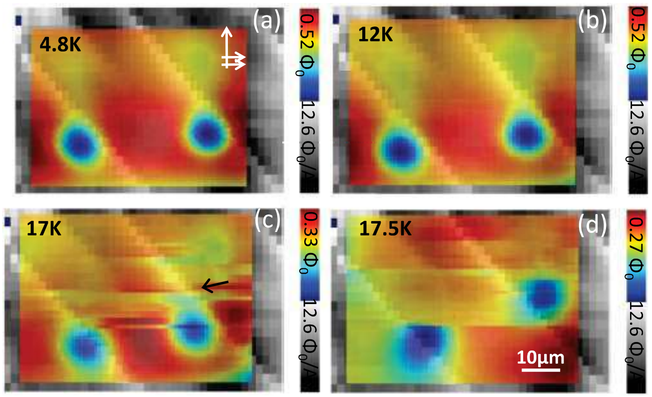


FIG. 3. Density plots of $\mathscr{H}$(panels (a) to (d)) and $|\tilde{\ }|^2$ (panels (e) to (f)) for $\hat{\lambda}_{2,-}$. The vortex begins at a distance 6← from the nematic domain wall and is attracted to it until it gets pinned. The vortex core is elongated before it gets pinned and this e↲ect gets enhanced once pinning happens.

Twin domain pining vs Nematic wall pining?





Behavior of vortices near twin boundaries in underdoped $Ba(Fe_{1-x}Co_x)_2As_2$

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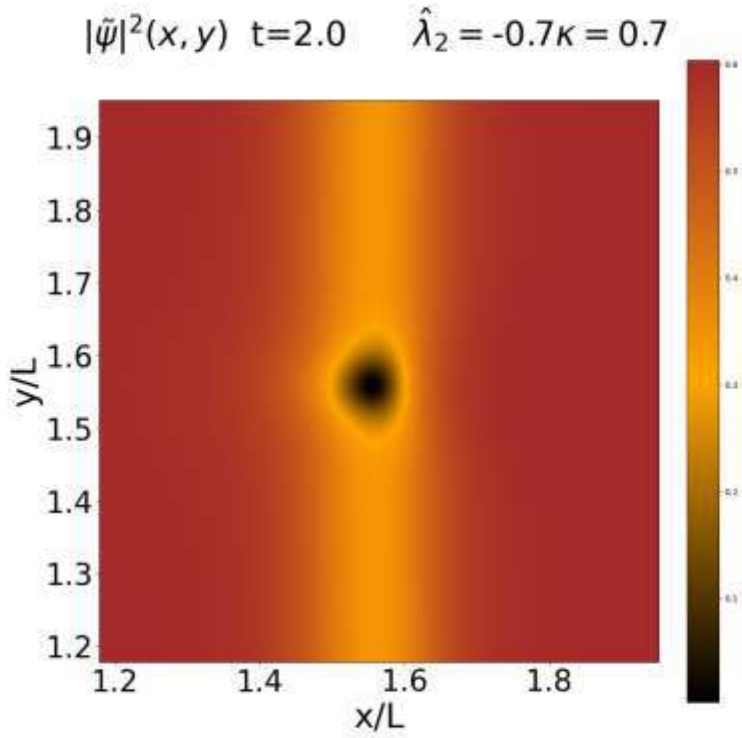
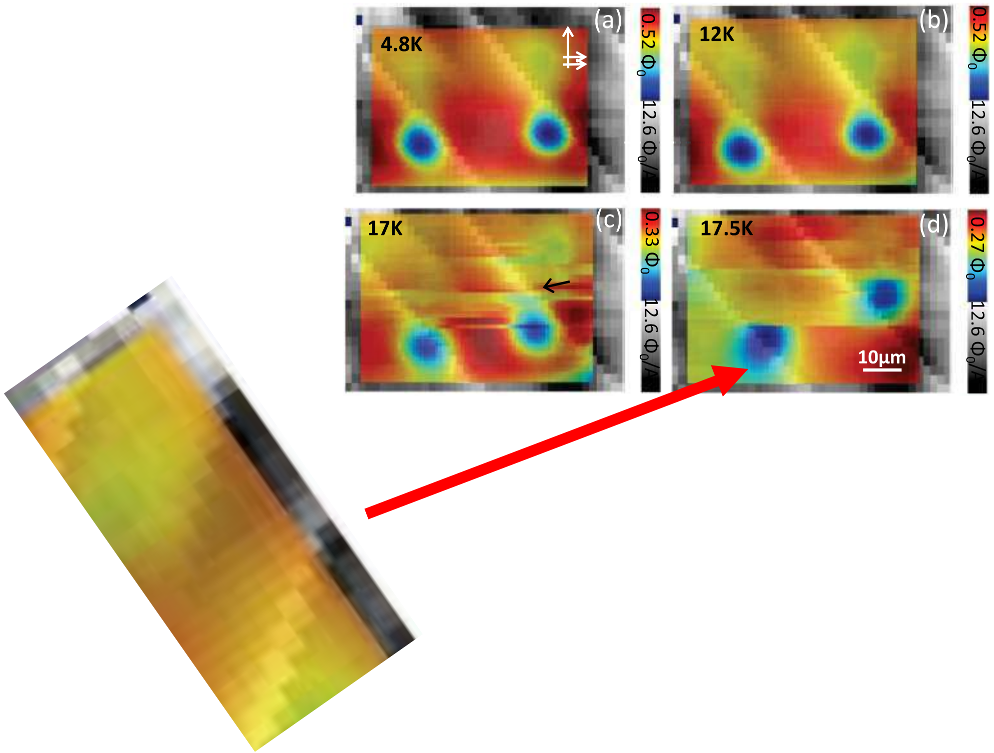
Vortex on the wall





Conclusions

1-We have studied the effect of nematicity in vortex-vortex interactions

2-We have implemented a new numerical method in the field of Superconductivity that allows to study time dependent phenomena more efficiently

3-The method is well suited to study other problems, like pining, disorder, temperature fluctuations

Thanks for your attention

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