



Self-organized topological superconductivity in Yu-Shiba-Rusinov chains

...and frustrated magnetism in YSR lattices



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Outline

1. From single Yu-Shiba-Rusinov states to YSR chains and Top-SC
2. Magnetic order of 1D chains in 3D SC
3. Interplay between magnetic order and Top-SC
4. Magnetic order of 1D chains in 2D SC (*Briefly*)
5. Magnetic order of 2D lattice in 3D SC

Collaborators

-Michael Schecter
-Morten Holm Christensen
-Karsten Flensberg
-Brian Møller Andersen
-Olav Fredrik Syljuåsen

Papers

Schecter *et al.*, PRB **93**, 140503(R) (2016)

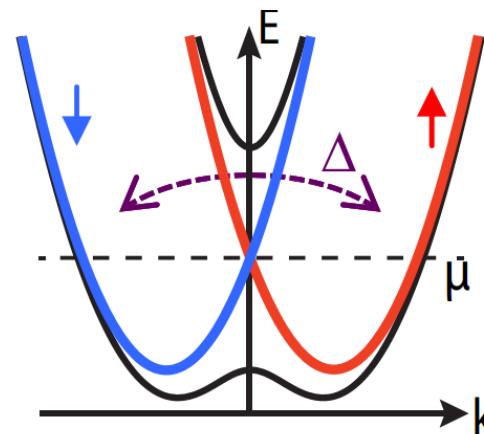
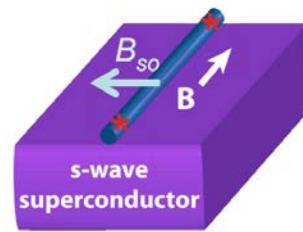
Christensen *et al.*, arXiv:1607.08190



The 1D topological superconductor

- Superconductor with localized, zero-energy q.p. excitations (Majorana)
- Simplest example: 1d spinless electrons with pairing
- InSb, InAs in proximity to Nb, or Al

Spin-orbit coupling
+
Orthogonal Zeeman field



$$H = \left(\frac{k^2}{2m} - \mu + \alpha k \sigma_z \right) \tau_z + \Delta \tau_x + B \sigma_x$$

- R. M. Lutchyn et al., PRL **105**, 077001 (2010)
Y. Oreg et al., PRL **105**, 177002 (2010)
V. Mourik et al., Science **336**, 1003 (2012)



Replacing SOI with spiraling B-fields or spins

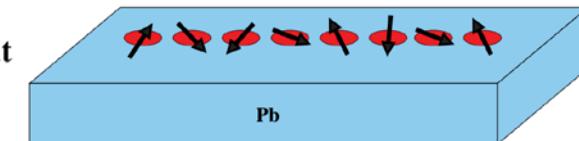
PHYSICAL REVIEW B 84, 195442 (2011)



Majorana

from magnetic nanoparticles on a superconductor without spin-orbit coupling

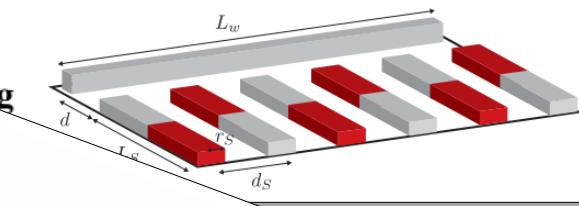
A. V. Ustinov, A. V. Chubukov, M. V. Feigel, V. V. Kozhevnikov, and C. W. J. Beenakker



PHYSICAL REVIEW B 88, 020407(R) (2013)

Majorana fermions in superconductors

S. Nadj-Perge, I. K. Drozdov, B. A. Bernevig, and Ali Yazdani*

Morten Kjaergaard,¹ Konrad Womacki,¹ and Bernd Braunecker¹

PRL 111, 147202 (2013)

PHYSICAL REVIEW LETTERS

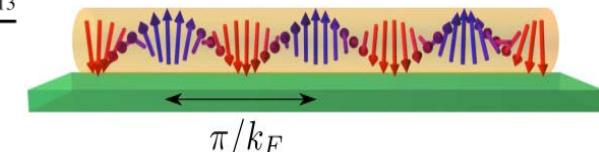
Interplay between Classical Magnetic Moments and Superconductivity in Quantum One-Dimensional Conductors: Toward a Self-Sustained Topological Majorana Phase

Bernd Braunecker¹

PRL 111, 186805 (2013)

PHYSICAL REVIEW B 88, 155420 (2013)

Topological superconducting phase in helical Shiba chains

Falko Pientka,¹ Leonid I. Glazman,² and Felix von Oppen¹week ending
NOVEMBER 2013

PHYSICAL REVIEW LETTERS

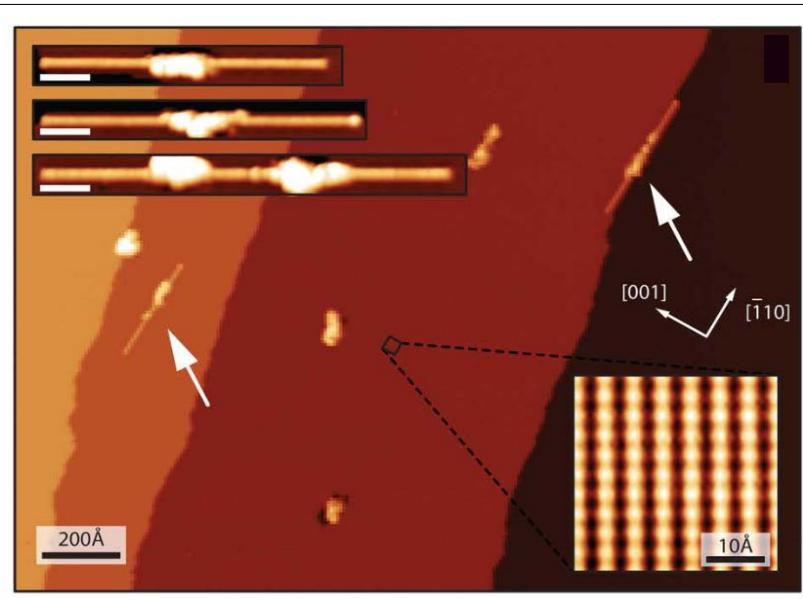
week ending
15 NOVEMBER 2013

Self-Organized Topological State with Majorana Fermions

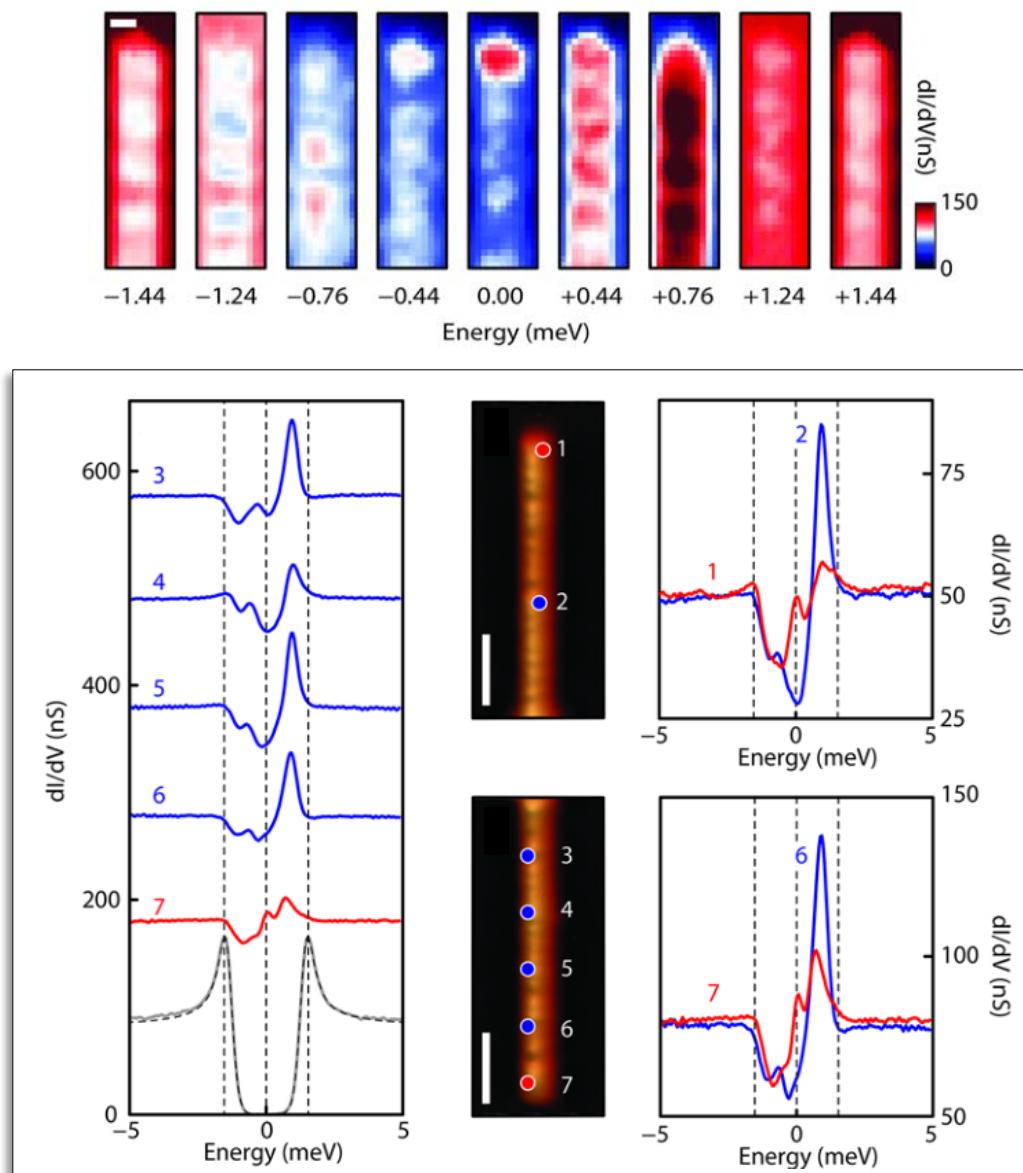
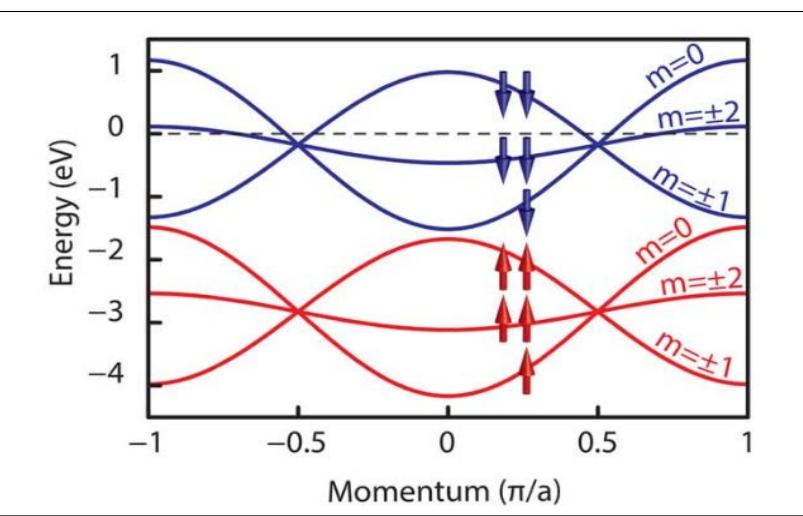
M. M. Vazifeh and M. Franz



Majorana bound states from Fe chains on Pb(110)



Nadj-Perge et al., Science **346**, 602 (2014)



Yu-Shiba-Rusinov states

BOUND STATE IN SUPERCONDUCTORS WITH
PARAMAGNETIC IMPURITIES

Yu Luh (Yu Lu)

Received July 10, 1963

Acta Physica Sinica 21, 75-91 (January, 1965)

Progress of Theoretical Physics, Vol. 40, No. 3, September 1968

Classical Spins in Superconductors

Hiroyuki SHIBA^{*)}

Dep.

SUPERCONDUCTIVITY NEAR A PARAMAGNETIC IMPURITY

A. I. Rusinov

P. N. Lebedev Physics Institute, USSR Academy of Sciences

Submitted 28 November 1968

ZhETF Pis. Red. 9, No. 2, 146-149 (20 January 1969)

It is shown that with a classical spin form an "impurity observable quantity"

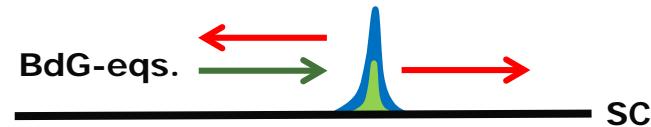
$$\omega = \pm \omega_B \equiv \pm \Delta_0 \frac{1 - ((J/2) S \pi \rho)^2}{1 + ((J/2) S \pi \rho)^2}$$

It is shown in [1] that introduction of a small amount ($\sim 1\%$) of paramagnetic impurities in a superconductor exerts a strong influence on its properties. In particular, the energy

lloy no longer coincides with the magnitude of the ordering [1] was carried out in the Born approximation with respect ill be shown below that in the case of a superconductor al of the scattering of the electrons by the magnetic impurity results.



Rusinov solution

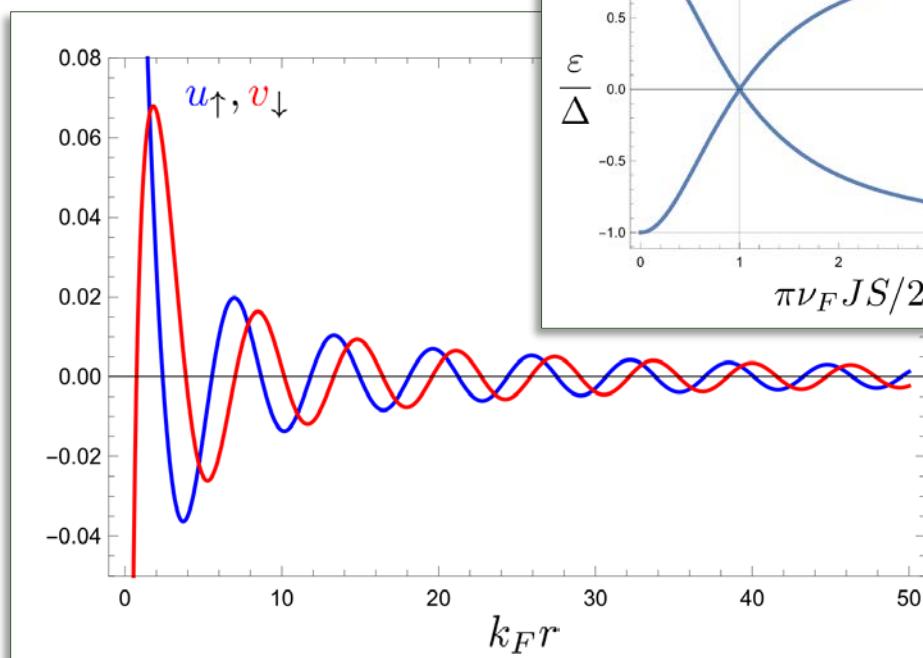
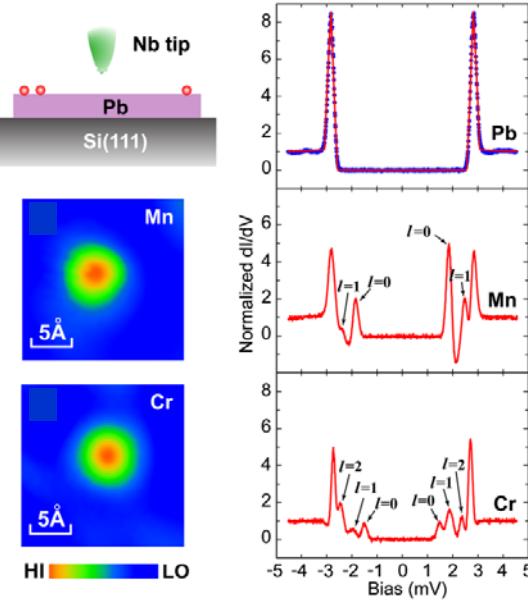


Spin-dependent δ -function potential: $V_\sigma(\mathbf{r}) = (U + JS\tau_{\sigma\sigma}^z)\delta(\mathbf{r})$

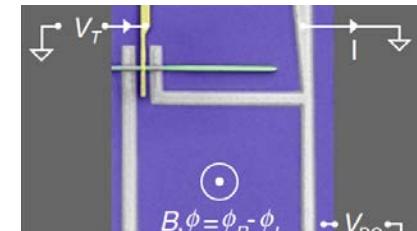
Eigenenergies: $\varepsilon = \Delta \frac{1 - (\pi\nu_F JS/2)^2}{1 + (\pi\nu_F JS/2)^2} = \Delta \cos(\delta^+ - \delta^-)$, $\tan(\delta^\pm) = \nu_F(U \pm JS)$

Eigenfunctions (3D): $\begin{pmatrix} u_\uparrow(\mathbf{r}) \\ v_\downarrow(\mathbf{r}) \end{pmatrix} = \frac{1}{\sqrt{c}} \frac{\sin(k_F r + \delta^\pm)}{k_F r} e^{-r/(\xi/|\sin(\delta^+ - \delta^-)|)}$

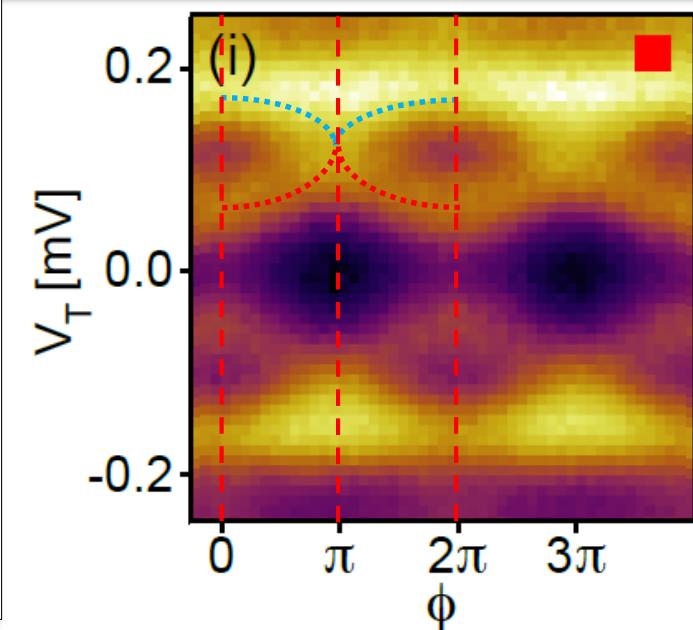
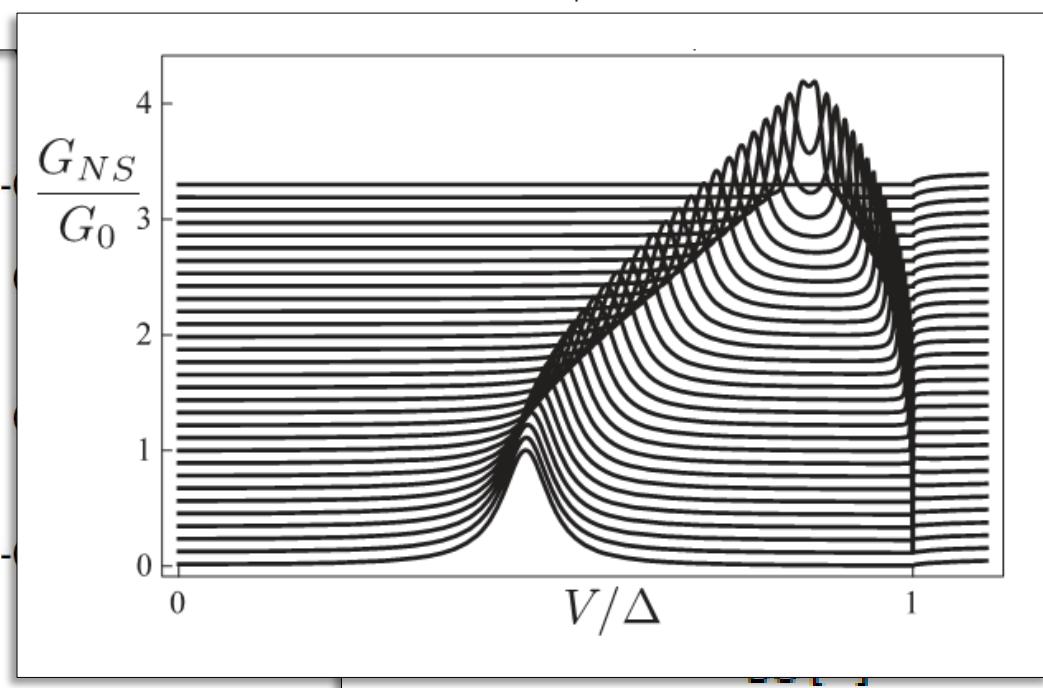
Ji et al., Science **100**, 226801 (2008)



YSR in quantum dots (2-channels, phase-bias)

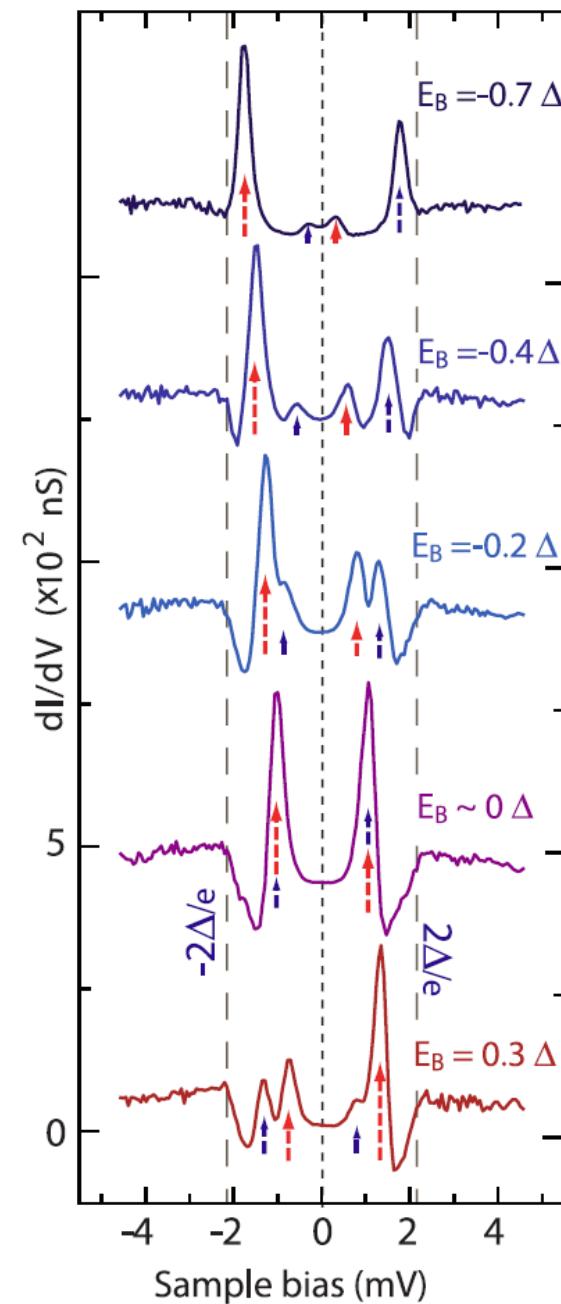
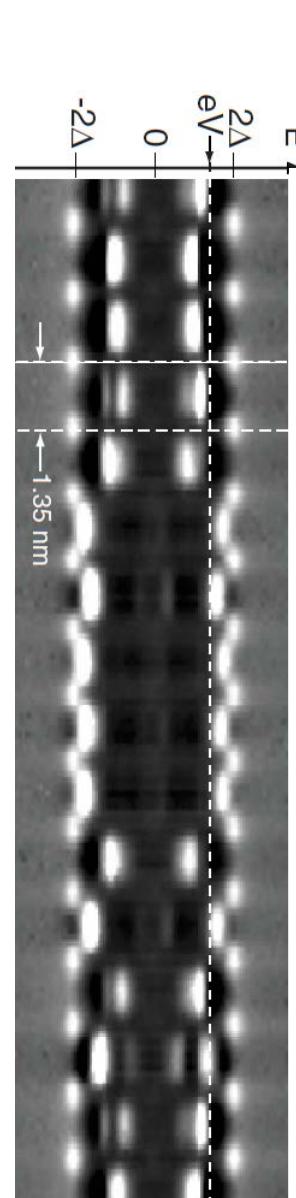
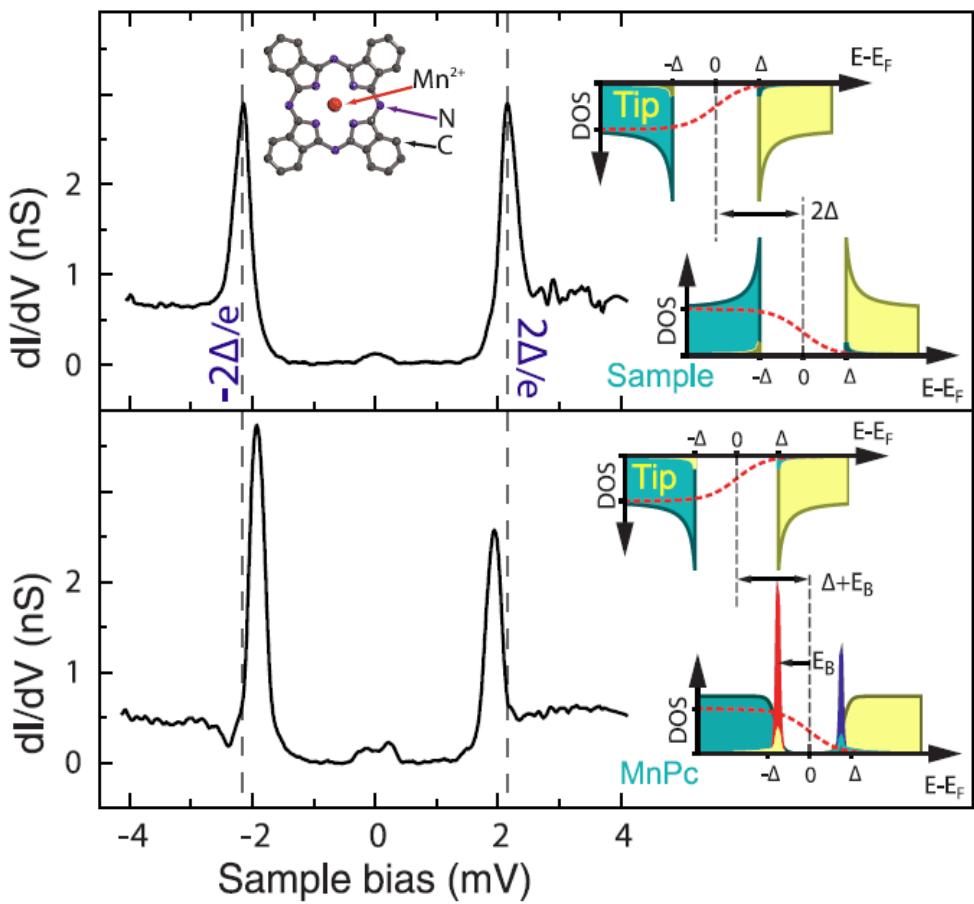


$$E^2 = \frac{|\Delta|^2}{(1+u^2)^2 + 4g^2} \left(1 - u^2(1+u^2) \sin^2(2\theta) \sin^2 \frac{\phi}{2} + 2w^2 + u^4 \pm g \sqrt{4g^2 + 4u^2[1+u^2 \cos^2(2\theta)] \sin^2(2\theta) \sin^2 \frac{\phi}{2} + u^4 \sin^4(2\theta) \sin^2 \phi} \right)$$



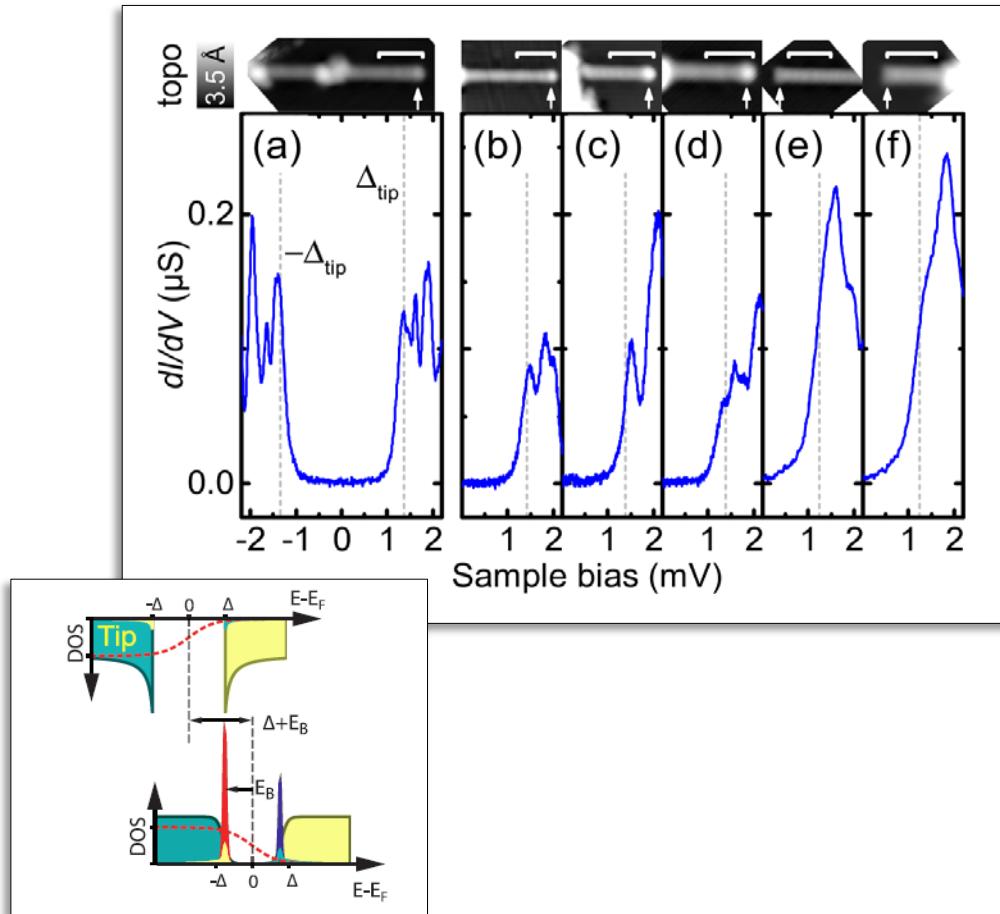
Pb-MnPc-Pb (STM, 2D spin-lattice)

K. J. Franke et al., Science **332**, 940 (2011)

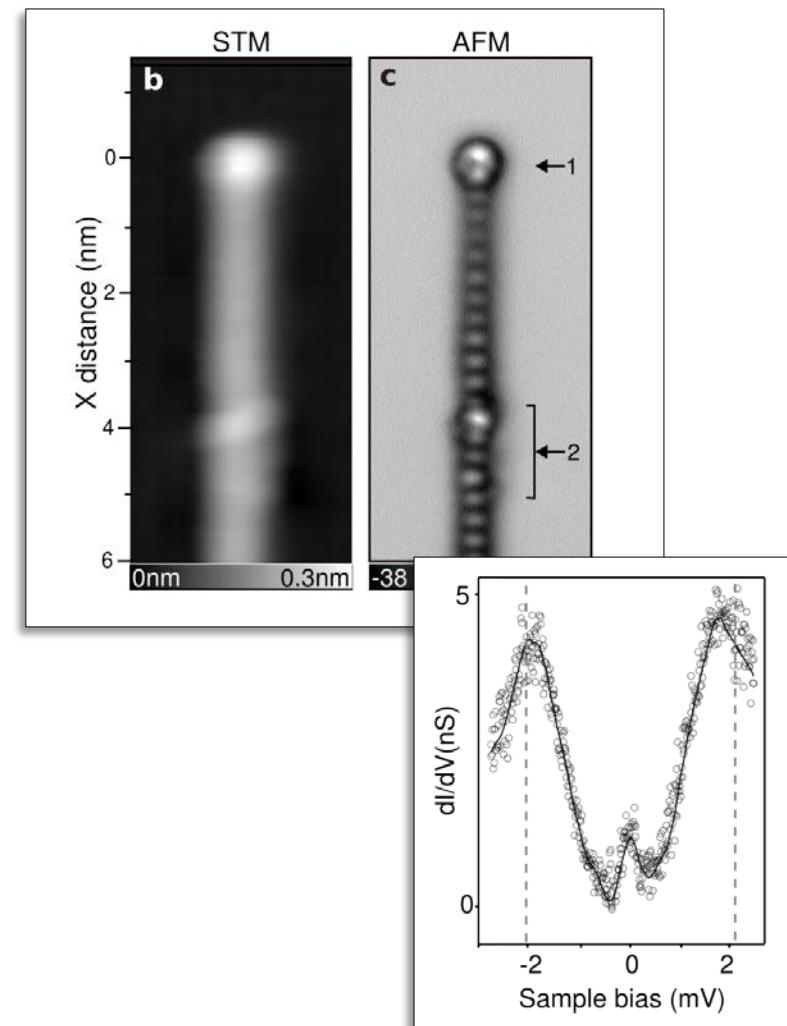


More zero-energy sub-gap states from **Fe** chains on **Pb**(110)

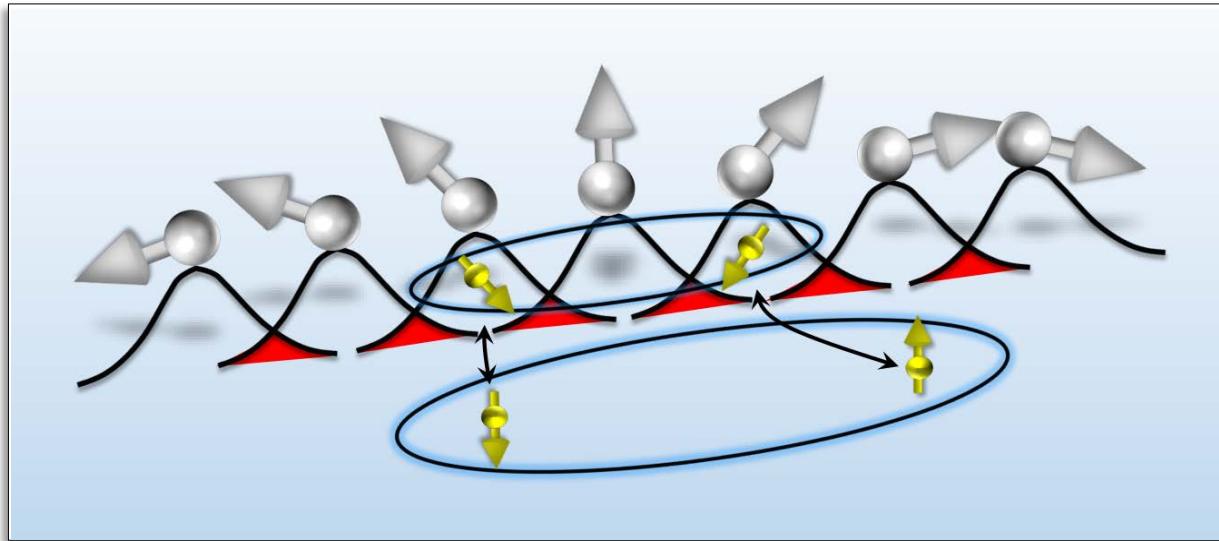
Ruby et al., PRL **115**, 197204 (2015)



Pawlak et al., arXiv: 1505.06078



The 1D classical spin chain in a 3D superconductor



$$H = \frac{1}{2} \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger (\xi_{\mathbf{k}} \tau_z + \Delta \tau_x) \Psi_{\mathbf{k}} + \frac{1}{2} J \int_{\mathbf{r}} \Psi_{\mathbf{r}}^\dagger \vec{S}_{\mathbf{r}} \cdot \boldsymbol{\sigma} \Psi_{\mathbf{r}}$$

$$\xi(\mathbf{k}) = \frac{\mathbf{k}^2 - k_F^2}{2m}$$

$$\Psi = (\psi_{\uparrow}, \psi_{\downarrow}, \psi_{\downarrow}^\dagger, -\psi_{\uparrow}^\dagger)^T$$

$$\vec{S}_r = S \sum_j \delta(r - ja) (\cos qr, \sin qr, 0)$$



The calculation

$$\mathcal{G}(ik_n, 0) = -\frac{\pi\nu_F}{2} \frac{ik_n\tau_0 + \Delta\tau_x}{\sqrt{k_n^2 + \Delta^2}} \sigma_0$$

$$\mathcal{T}(ik_n) = J\sigma_x \left(1 + \frac{\pi J\nu_F}{2} \frac{ik_n\tau_0 + \Delta\tau_x}{\sqrt{k_n^2 + \Delta^2}} \sigma_x \right)^{-1} \quad (\text{YSR's as poles in T-matrix})$$

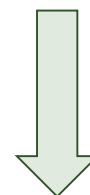
$$\mathcal{G}(ik_n, r) = -\frac{\pi\nu_F}{2} \frac{e^{-r\sqrt{k_n^2 + \Delta^2}/v_F}}{k_F r} \sigma_0 \left[\frac{ik_n\tau_0 + \Delta\tau_x}{\sqrt{k_n^2 + \Delta^2}} \sin(k_F r) + \tau_z \cos(k_F r) \right]$$

$$\tilde{\mathcal{G}}(i\omega, k) = \sum_{j \neq 0} \mathcal{G}(i\omega, ja) e^{-ikaj} \quad (\text{Fourier series along transl. inv. chain})$$

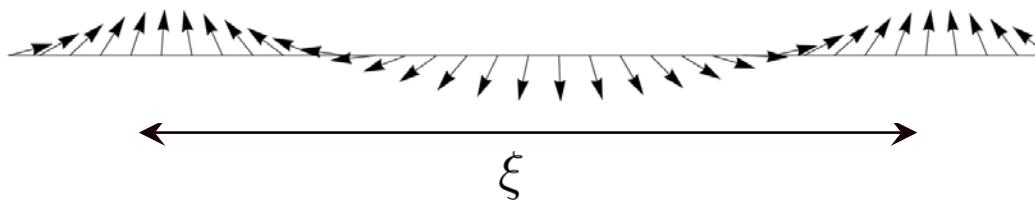
$$E(q) = -\frac{Na}{2} \int \frac{d\omega}{2\pi} \frac{dk}{2\pi} \text{Tr} \ln \left[1 - \tilde{\mathcal{G}}(i\omega, k - \frac{1}{2}q\sigma_z)\mathcal{T} \right]$$

$$\approx \frac{1}{4} \sum_{i \neq j} \int \frac{d\omega}{2\pi} \text{Tr} [\mathcal{T}_i \mathcal{G}_{0,ij} \mathcal{T}_j \mathcal{G}_{0,ji}] \quad (\text{Effective Heisenberg exchange})$$

To 2nd order in J : Weak instability of FM



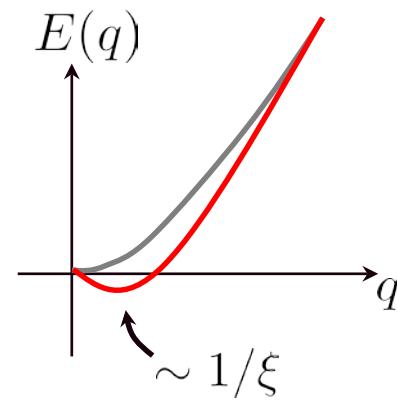
Anderson & Suhl, Phys. Rev. **116**, 898–900 (1959)
 Abrikosov, "Fundamentals of the theory of metals", (1988)
 Aristov et al., Z. Phys. B **102**, 467–471 (1997)



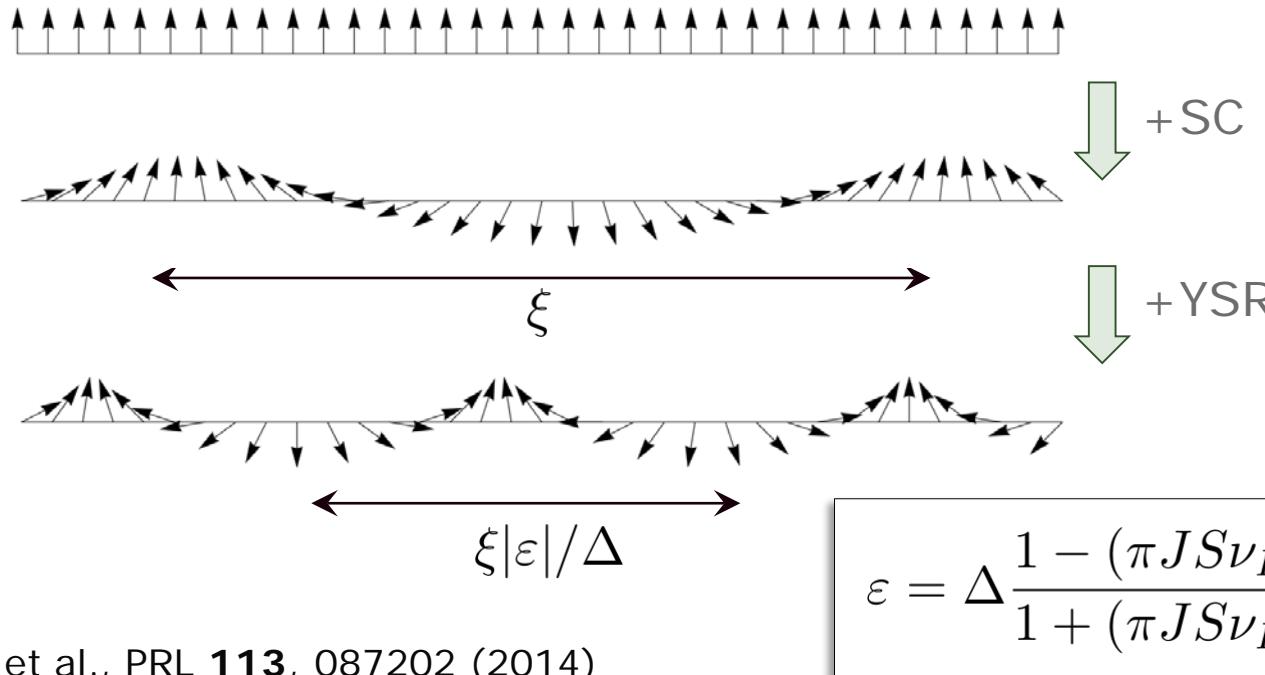
BCS-modified RKKY-interaction:

$$I(r) \propto J^2 e^{-2r/\xi} \left[\frac{v_F}{2\pi r^3} \cos(2k_F r) + \frac{\Delta}{r^2} \sin^2(k_F r) \right]$$

$v_F = \xi \Delta$



To 2nd order in \mathcal{T} : More pronounced spiral order



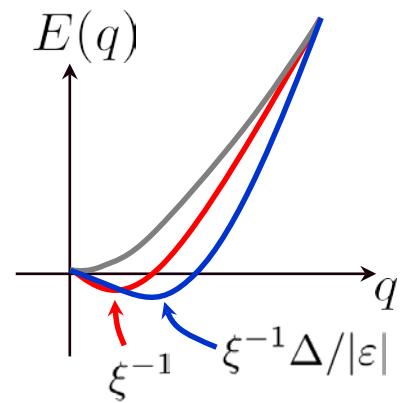
$$\varepsilon = \Delta \frac{1 - (\pi JS\nu_F/2)^2}{1 + (\pi JS\nu_F/2)^2}$$

Yao et al., PRL 113, 087202 (2014)

YSR/BCS-modified interaction:

$$I(r) \propto J^2 e^{-2r/\xi} \left[\frac{v_F}{2\pi r^3} \cos(2k_F r) + \frac{\Delta}{r^2} \sin^2(k_F r) \right]$$

$$I(r) \propto \left(1 - \frac{\varepsilon^2}{\Delta^2}\right) e^{-2r/\xi} \left[\frac{v_F}{2\pi r^3} \cos(2k_F r) + \frac{\Delta^2 \cos^2(k_F r)}{2|\varepsilon|r^2} + \frac{|\varepsilon|}{4r^2} [1 - 3\cos(2k_F r)] \right]$$



YSR band-structure

YSR-band from 4 poles of Green fct.:

$$\begin{aligned} 0 &= \det \left[\tilde{\mathcal{G}}(\omega, k - q\sigma_z/2) - \mathcal{T}^{-1}(\omega) \right] \\ &= \det \left[\tilde{B}\sigma_x + \frac{\omega + \Delta\tau_x}{\sqrt{\Delta^2 - \omega^2}} (\tilde{\Delta}_s + \tilde{\Delta}_t\sigma_z) + (\tilde{\xi} + \tilde{\alpha}\sigma_z)\tau_z \right] \end{aligned}$$

$$\begin{aligned} \tilde{\xi} &= \text{Re } g_e(\omega, k) & \tilde{\alpha} &= \text{Re } g_o(\omega, k) \\ \tilde{\Delta}_s &= 1 + \text{Im } g_e(\omega, k) & \tilde{\Delta}_t &= \text{Im } g_o(\omega, k) \end{aligned}$$

$$\begin{aligned} \tilde{B} &= (\pi J\nu_F/2)^{-1} \\ &= \sqrt{(\varepsilon + \Delta)/(\varepsilon - \Delta)} \end{aligned}$$

$$\begin{aligned} g_{e/o}(\omega, k) = & -\frac{1}{2k_F a} \left[\ln(1 - e^{-(a/\xi)\sqrt{1-\omega^2/\Delta^2} + i(k_F + k - q/2)a}) \right. \\ & \left. + \ln(1 - e^{-(a/\xi)\sqrt{1-\omega^2/\Delta^2} + i(k_F - k + q/2)a}) \pm (k \rightarrow -k) \right] \end{aligned}$$

Compare to Y. Oreg et al., PRL **105**, 177002 (2010):

$$H = (\xi_k + \alpha k \sigma_z) \tau_z + \Delta \tau_x + B \sigma_x$$



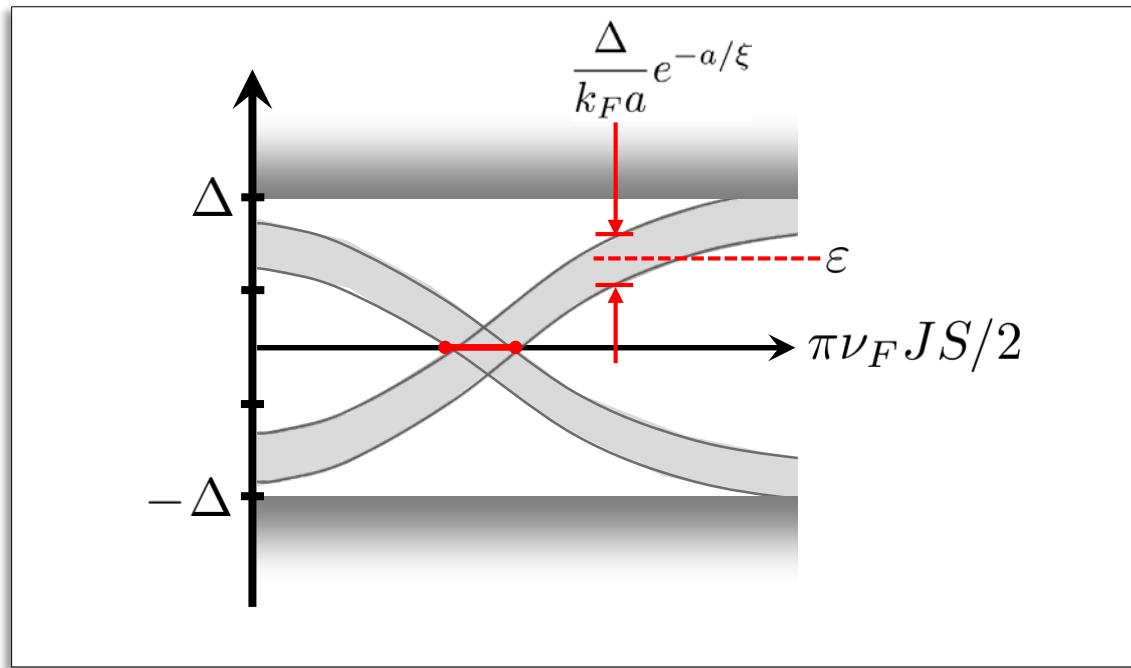
Limit of low-lying YSR states ($\varepsilon \ll \Delta$)

Expand to 2nd order in $\varepsilon/\Delta \ll 1 \ll k_F a$ gives the two lowest-lying bands:

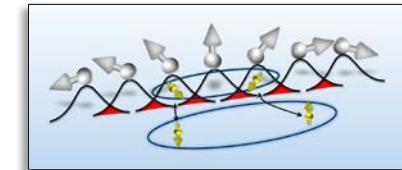
$$E_k = \sqrt{(h_k - \varepsilon)^2 + \Delta_k^2}$$

$$\begin{aligned} h_k &= \Delta \text{Im } g_e(0, k) \\ \Delta_k &= -\Delta \text{Re } g_o(0, k) \end{aligned}$$

Pientka et al. PRB **88**
155420 (2013)



Limit of low-lying YSR states ($|\varepsilon| < \Delta/(k_F a)$)



YSR contribution to total energy: $E_{\text{YSR}} = -\frac{1}{2} \sum_k E_k$ (Minimize, varying q)

Two competing effects:

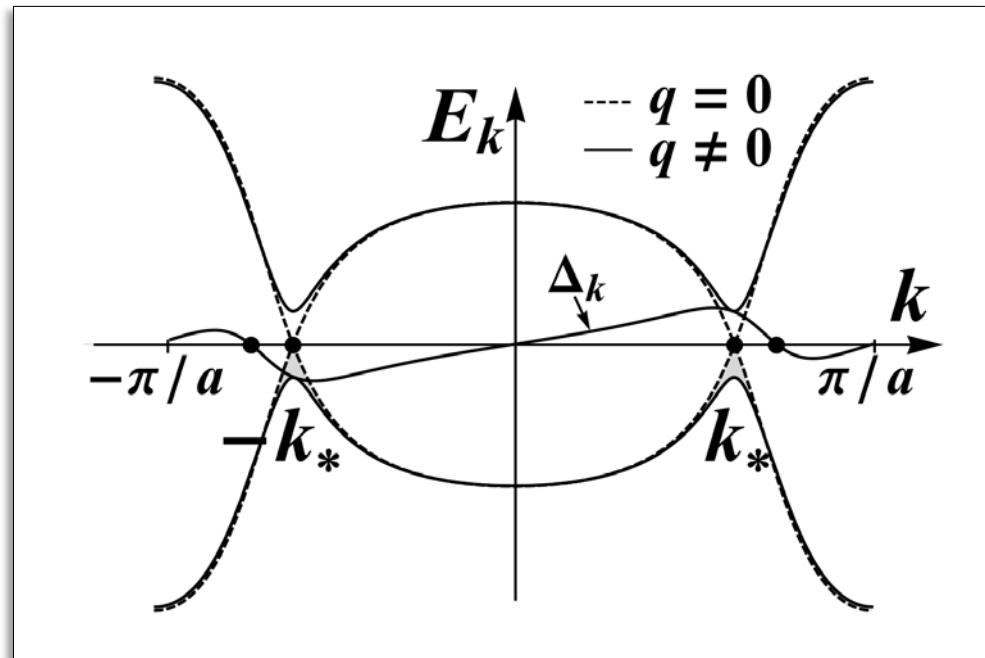
- I. Double-exchange (FM): Maximize kinetic energy by aligning spins, gapless
- II. Cooper-pair tunneling (spiral): Needs non-aligned spins, gap $\propto q$

I. (FM) only wins at critical line:

$$\varepsilon_c = \frac{\Delta}{k_F a} [\pi/2 - (k_F a \bmod \pi)]$$

II. (Spiral) wins elsewhere with:

$$\frac{qa}{\pi} = \left| \frac{\Delta/k_F a}{\varepsilon - \varepsilon_c} \right| e^{-\left(\frac{\Delta/k_F a}{\varepsilon - \varepsilon_c}\right)^2}$$



Topological YSR superconductor ($|\varepsilon| < \Delta/(k_F a)$)

Topological Hamiltonian:

$$\begin{aligned} H_t(k) &= \tilde{\mathcal{G}}(0, k - \frac{1}{2}q\sigma_z) - \mathcal{T}^{-1}(0) \\ &= \tilde{B}\sigma_x + \tilde{\xi}\tau_z + \tilde{\alpha}\sigma_z\tau_z + \tilde{\Delta}_s\tau_x + \tilde{\Delta}_t\sigma_z\tau_x \end{aligned}$$

Symmetries:

PH	$\Xi H_t(k)\Xi^{-1} = -H_t(-k)$	$\Xi = \sigma_y\tau_y\mathcal{K}$	$\Xi^2 = 1$
T (hidden)	$\mathcal{O}H_t(k)\mathcal{O}^{-1} = H_t(-k)$	$\mathcal{O} = -i\sigma_x\mathcal{K}$	$\mathcal{O}^2 = 1$
CHIRAL	$\{\mathcal{C}, H_t(k)\} = 0$	$\mathcal{C} = \mathcal{O}\Xi = \sigma_z\tau_y$	$\mathcal{C}^2 = 1$

→ Class BDI, with \mathbb{Z} -invariant $W = \frac{1}{2\pi i} \oint_{BZ} dk \partial_k \ln z(k)$

Gap closings at TRI momenta:

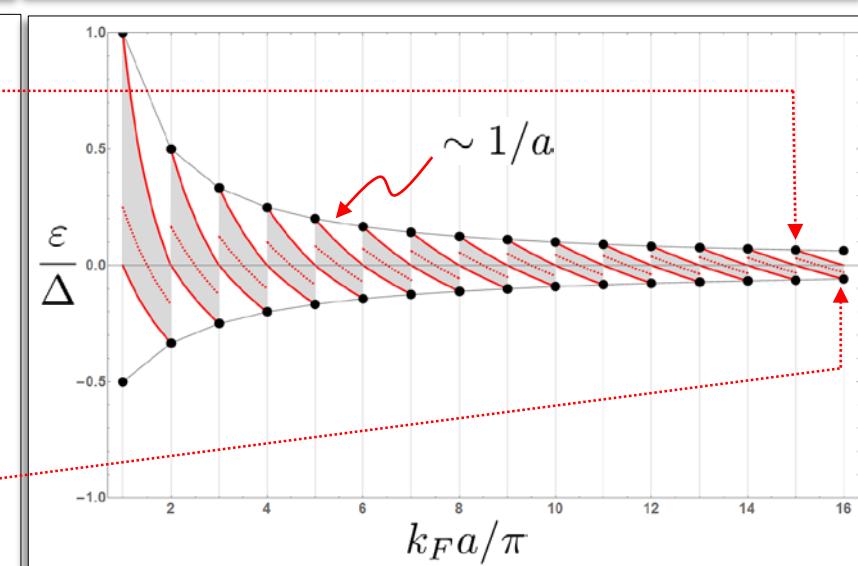
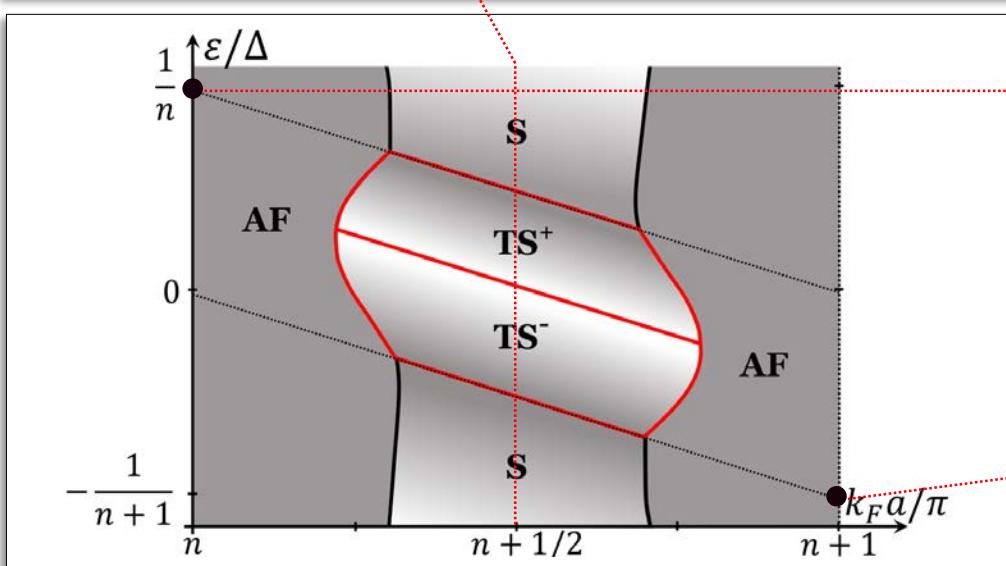
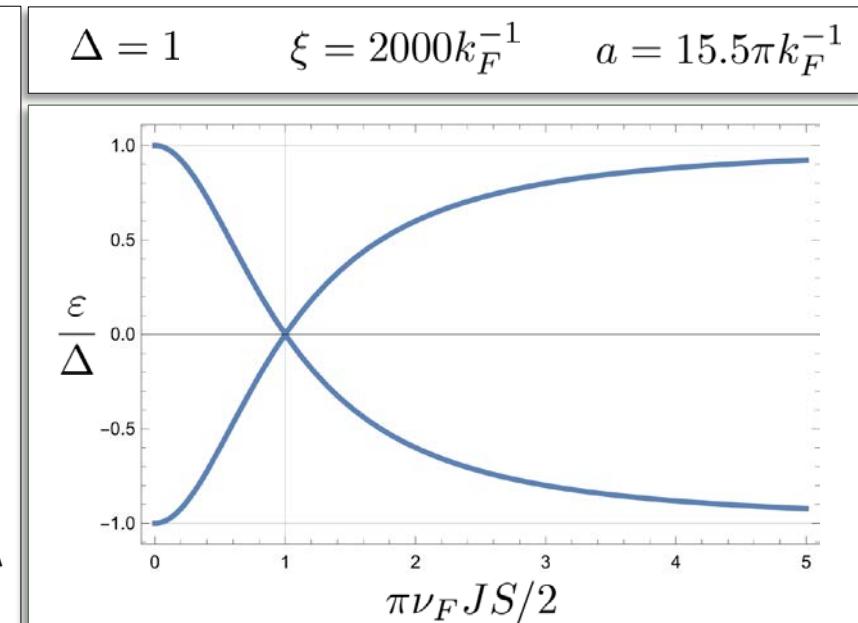
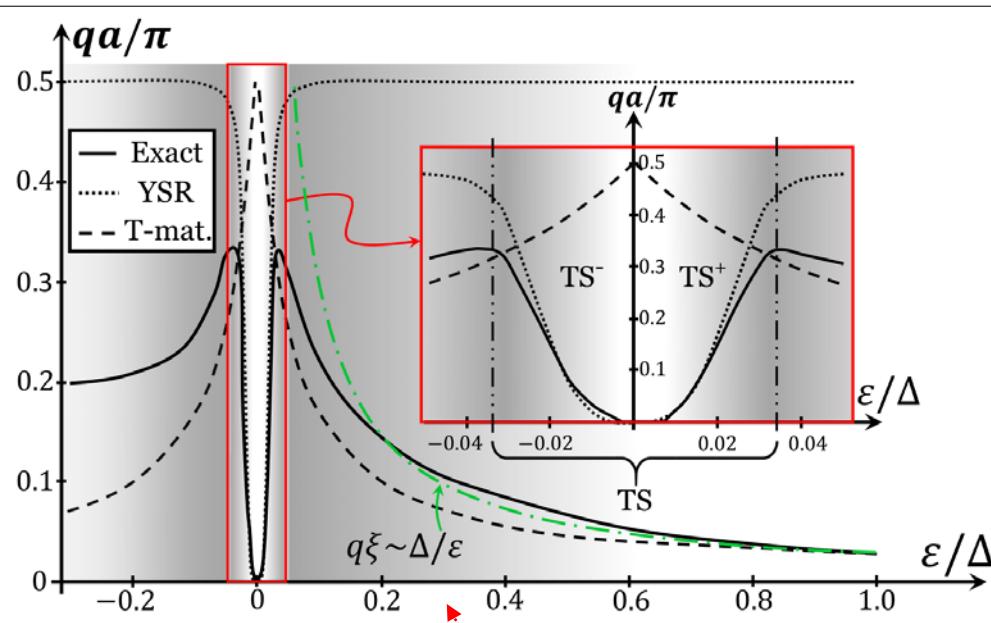
$$\frac{\varepsilon^\pm}{\Delta} \approx -(k_F a \bmod \mp \pi)/k_F a$$

$$z(k) = \det A / |\det A|$$

$$U^\dagger H_t U = \begin{pmatrix} 0 & A \\ A^\dagger & 0 \end{pmatrix}$$



Summarizing



Experimental considerations

Optimizing the topological gap:

$$\Delta_{top} \sim qa \frac{\Delta}{k_F a} \lesssim \frac{\Delta}{k_F a} \quad \text{max for } qa \sim 1$$

$$q \sim \xi^{-1} \frac{\Delta}{\varepsilon} \lesssim \frac{k_F a}{\xi} \quad \rightarrow \quad k_F a \sim \sqrt{k_F \xi} \quad \rightarrow$$

↑
Broad max at
 $\xi \sim 2000 k_F^{-1}$
 $a \sim 14.5 \pi k_F^{-1}$

Q&A:

1. Magnetic anisotropy: $H_D = -D \sum_{j=1}^N (S_j^z)^2$, harmless for $D < 0$
2. Spin-orbit coupling: ‘Gauges away into the spiral’
3. Self-consistent pairing potential: Not relevant for $k_F \gg 1/a, 1/\xi$
4. Fluctuations: Frozen out for $T \lesssim \max \left\{ D, \frac{S}{\ln N} \frac{\Delta}{k_F a} \right\}$
5. Quantum spins: From YSR, to Kondo lattice only when $\Delta \lesssim T_K$

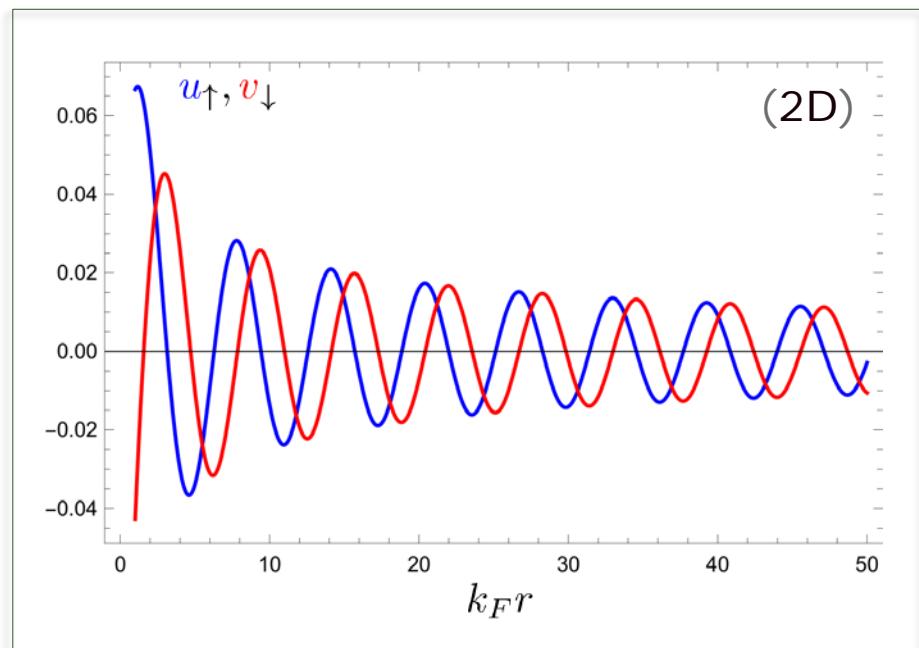
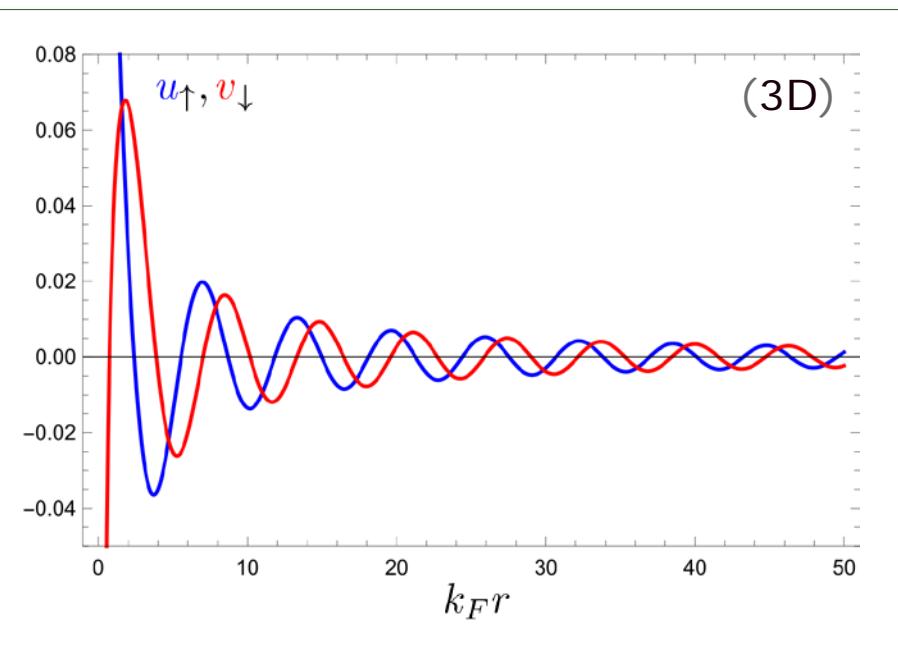


1D spin chain in 2D superconductor

Eigenfunctions (3D):
$$\begin{pmatrix} u_{\uparrow}(\mathbf{r}) \\ v_{\downarrow}(\mathbf{r}) \end{pmatrix} = \frac{1}{\sqrt{c}} \frac{\sin(k_F r + \delta^{\pm})}{k_F r} e^{-r/(\xi/|\sin(\delta^+ - \delta^-)|)}$$

Eigenfunctions (2D):
$$\begin{pmatrix} u_{\uparrow}(\mathbf{r}) \\ v_{\downarrow}(\mathbf{r}) \end{pmatrix} = \frac{1}{\sqrt{c}} \frac{\sin(k_F r - \frac{\pi}{4} + \delta^{\pm})}{\sqrt{\pi k_F r}} e^{-r/(\xi/|\sin(\delta^+ - \delta^-)|)}$$

Larger YSR hybridization expected in 2D:



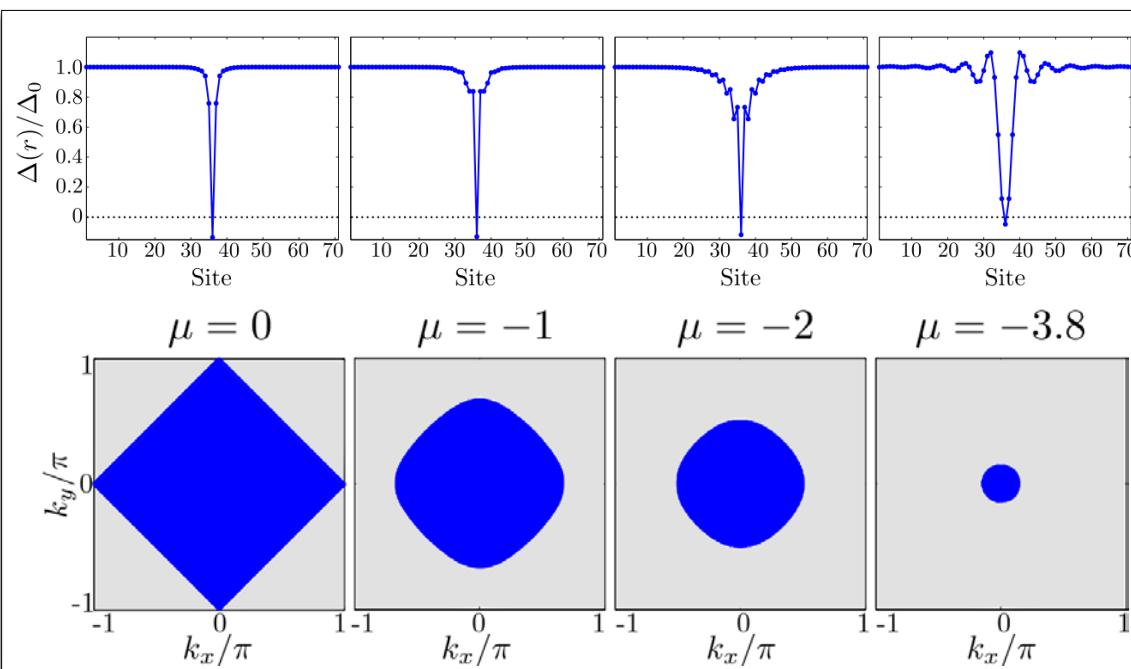
1D spin chain in 2D superconductor

$$H = - \sum_{\langle ij \rangle} (t_{ij} + \mu \delta_{ij}) c_{i\alpha}^\dagger c_{j\alpha} - V \sum_i n_{i\uparrow} n_{i\downarrow} + J \sum_{\substack{i \in I \\ \alpha\beta}} \mathbf{S}_i \cdot c_{i\alpha}^\dagger \boldsymbol{\tau}_{\alpha\beta} c_{i\beta}$$

$$H_{\text{SC}}^{\text{MF}} = - \sum_i \left[\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + h.c - \frac{|\Delta_i|^2}{V} \right]$$

$$\Delta_i = V \langle c_{i\downarrow} c_{i\uparrow} \rangle$$

BCS mean-field
decoupling

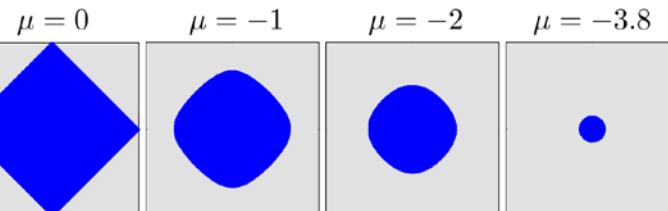
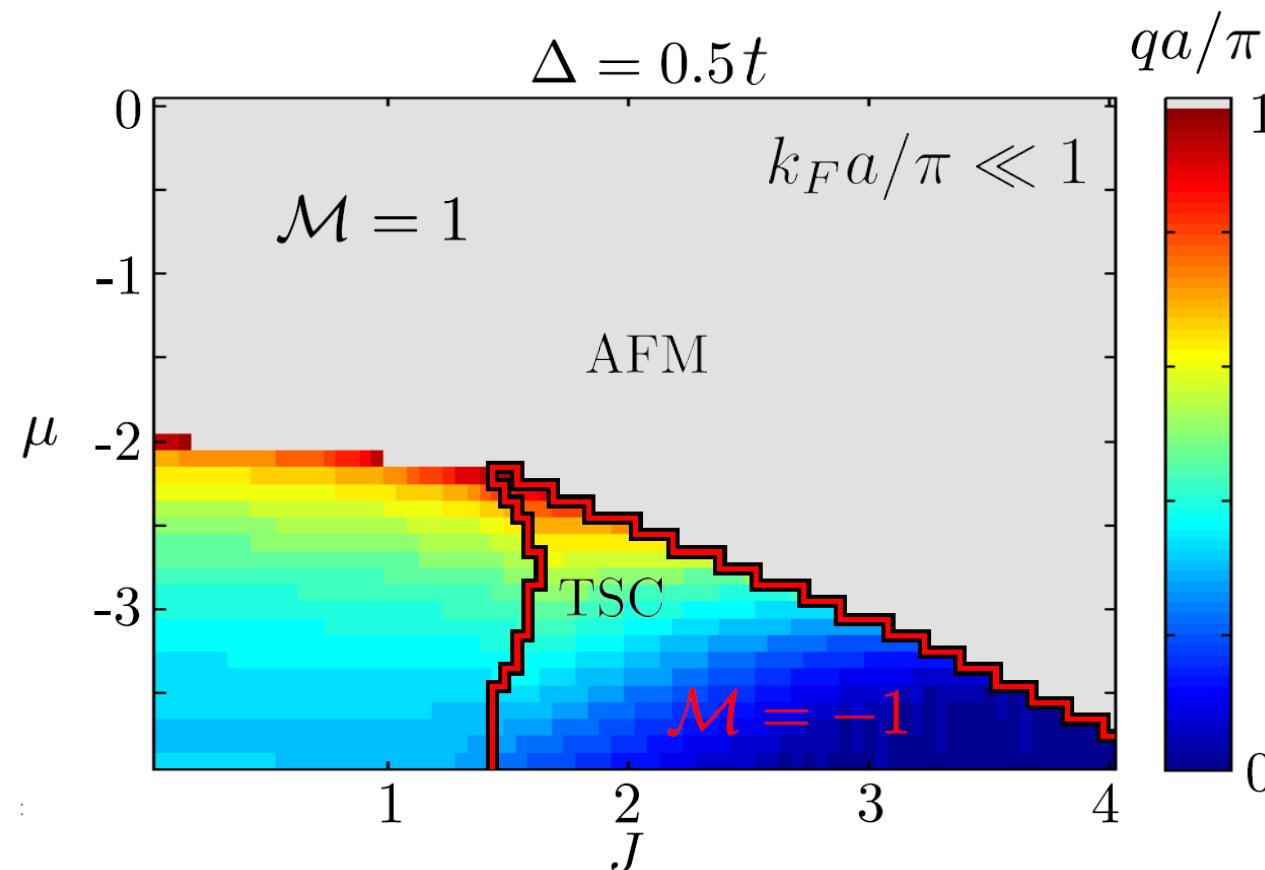


Local pairing
Potential

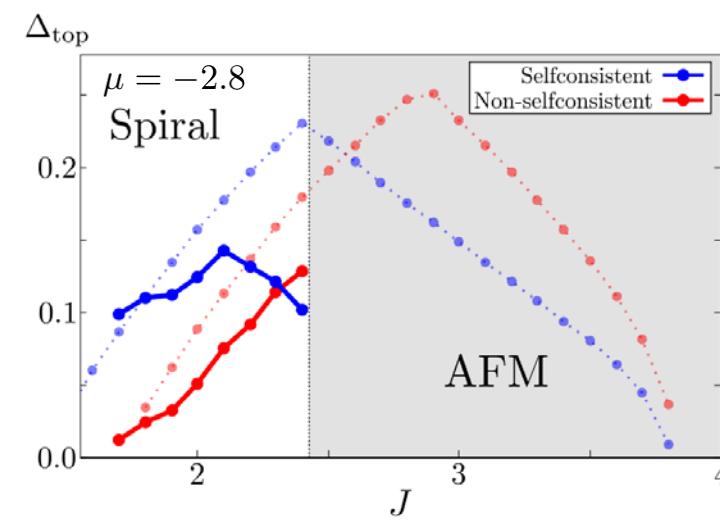
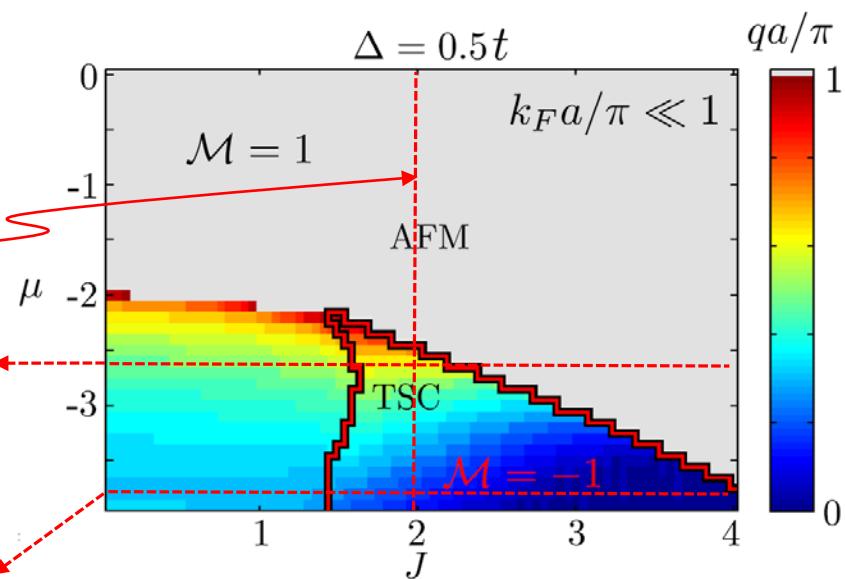
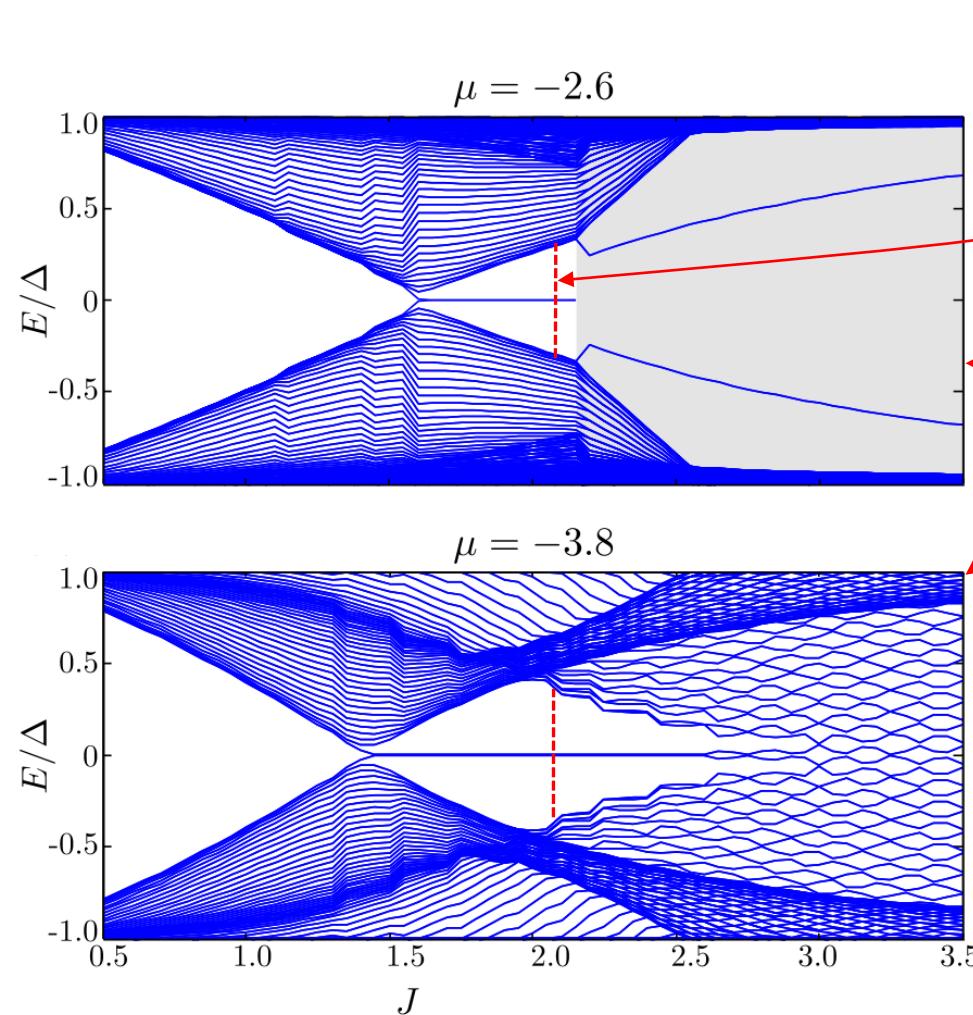
Evolution of
Fermi surfaces
with μ



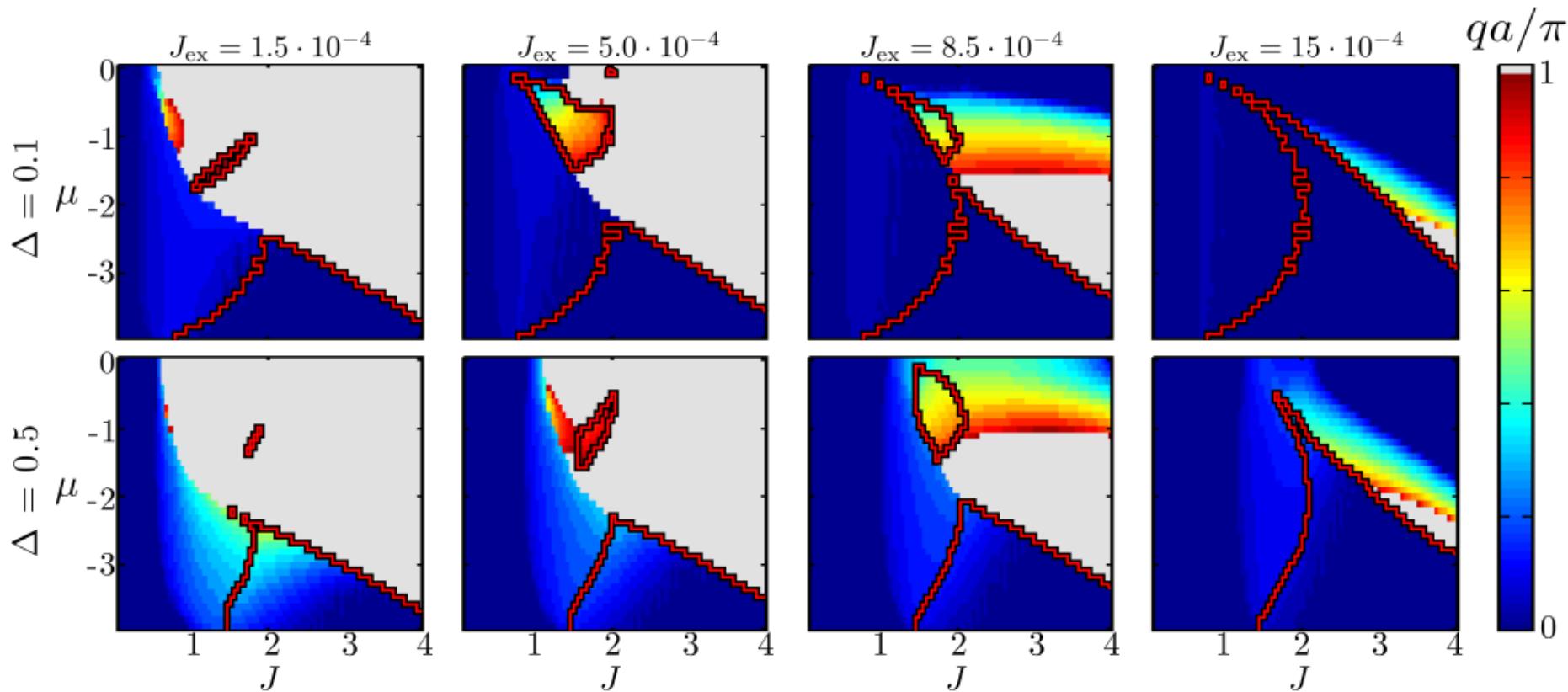
1D spin chain in 2D superconductor: Phase-diagram



YSR bands and Majorana bound states



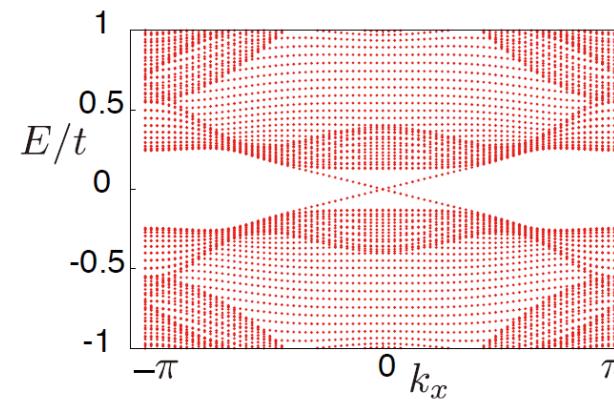
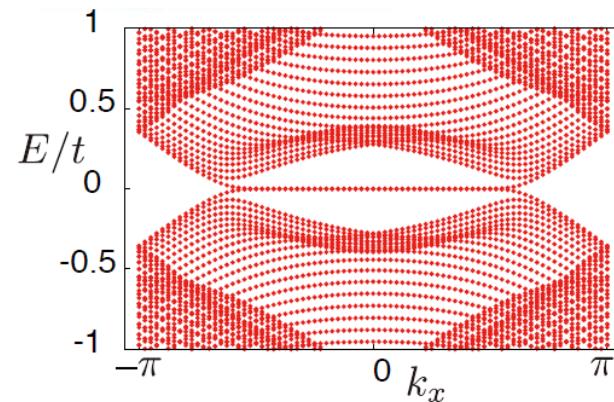
Including direct nearest neighbor FM exchange



2D spin lattice in 3D superconductor

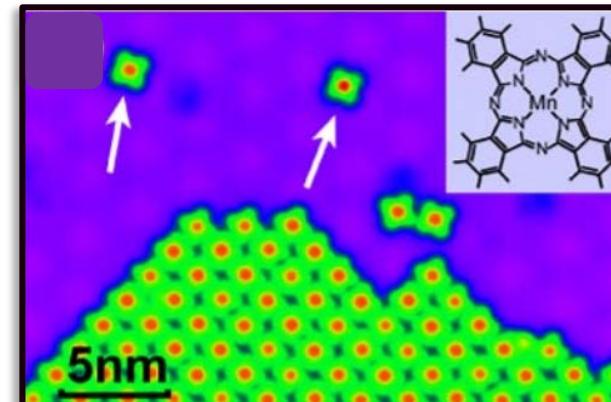
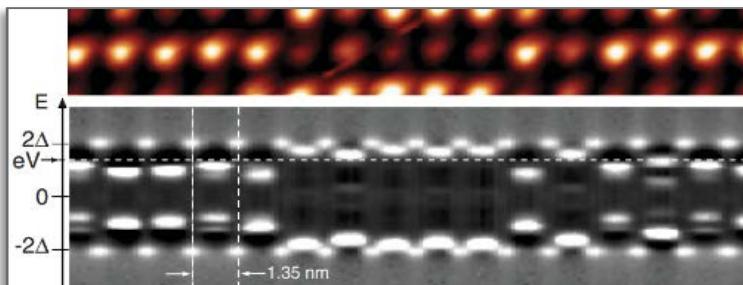
Noncollinear/noncoplanar magnetism may give rise to a
2D nodal/chiral p-wave YSR superconductor

S. Nakosai, Y. Tanaka, N. Nagaosa, PRB **88**, 180503(R) (2013)

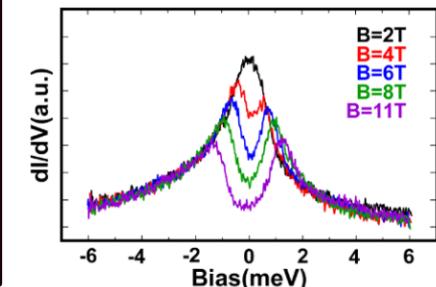


Square lattice of Mn-PC on Pb(111)

K. J. Franke et al.,
Science **332**, 940 (2011)



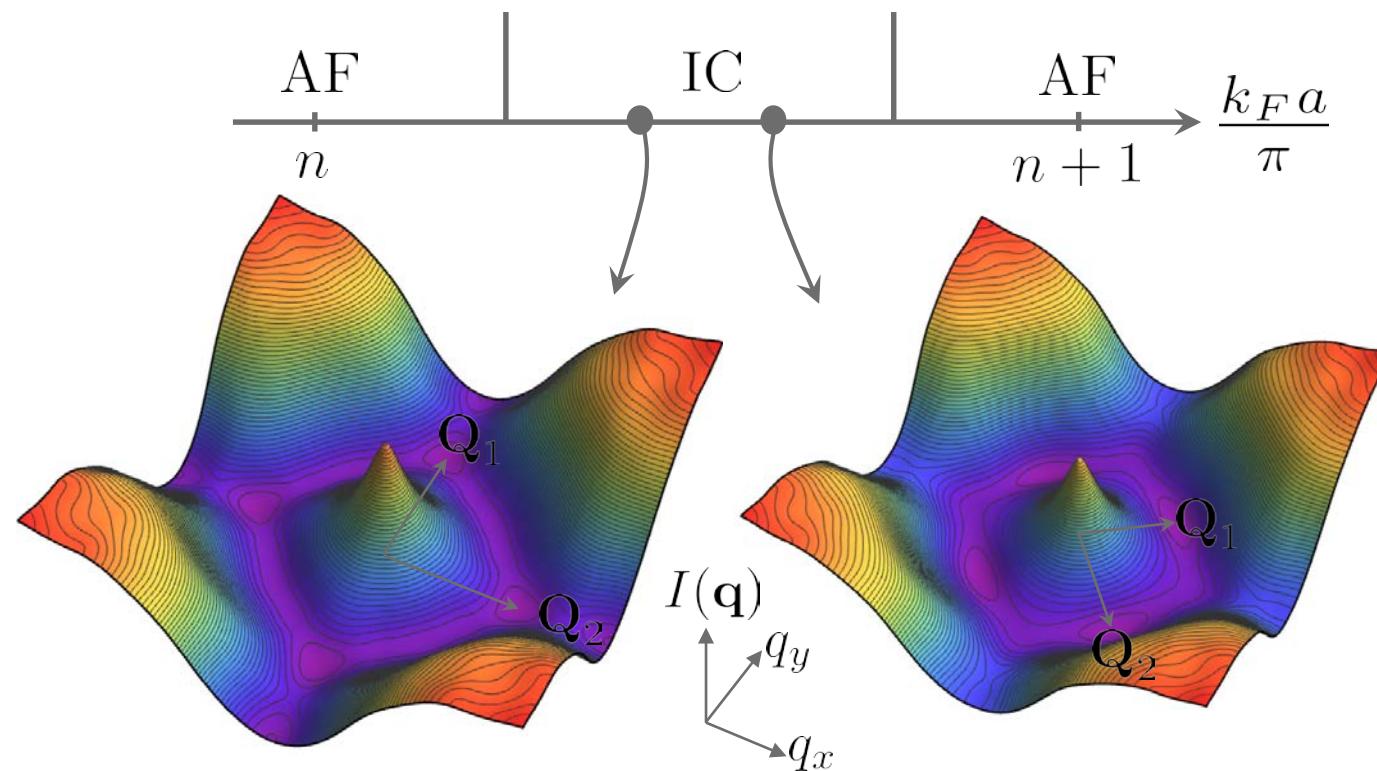
Y.S. Fu et al.,
PRL **99**, 256602 (2007)



Isotropic **BCS+YSR**-modified RKKY interaction (2D Fourier Transf.)

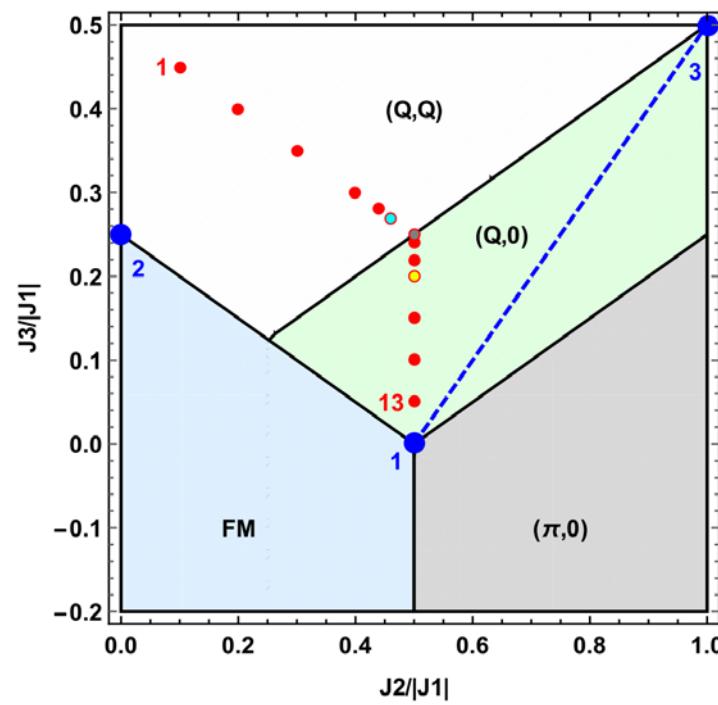
$$I(r) \propto \left(1 - \frac{\varepsilon^2}{\Delta^2}\right) \frac{e^{-2r/\xi}}{(k_F r)^{d-1}} \left[\frac{\Delta^2 + \varepsilon^2}{4|\varepsilon|} + \left(\frac{v_F}{2\pi r} + \frac{\Delta^2}{4|\varepsilon|} - \frac{3|\varepsilon|}{4} \right) \cos(2k_F r + (3-d)\pi/2) \right]$$

$$\mathcal{H}_{\text{Heis}} = \sum_{i,j} I_{(i-j)} \mathbf{S}_i \cdot \mathbf{S}_j = \sum_Q I_Q |\mathbf{S}_Q|^2$$

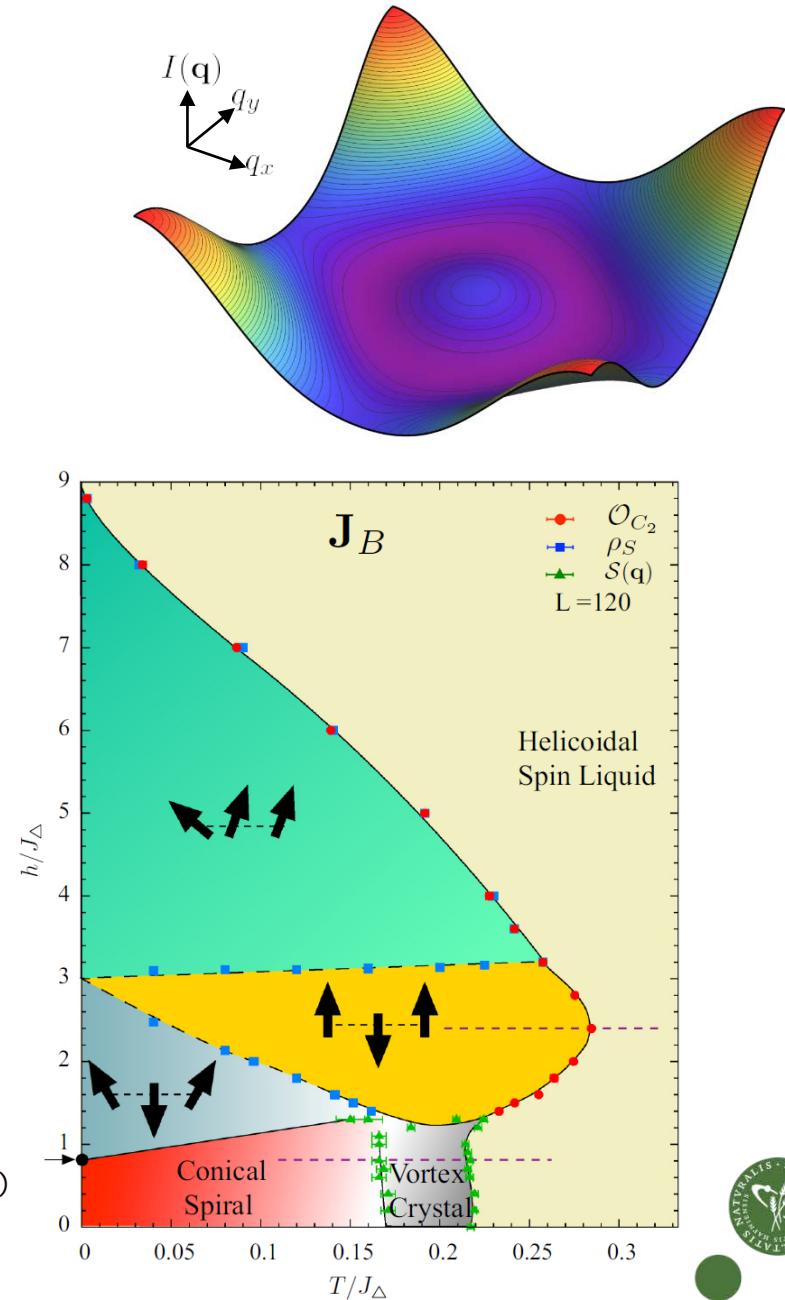


Ferromagnetic J_1 - J_2 - J_3 Toy Model

$$H = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j + J_3 \sum_{\langle\langle\langle ij \rangle\rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$

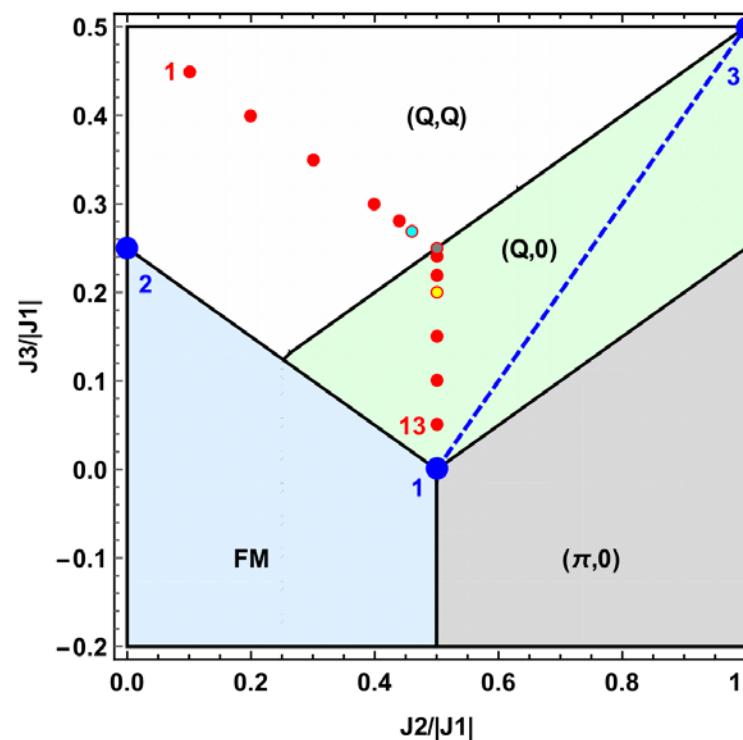
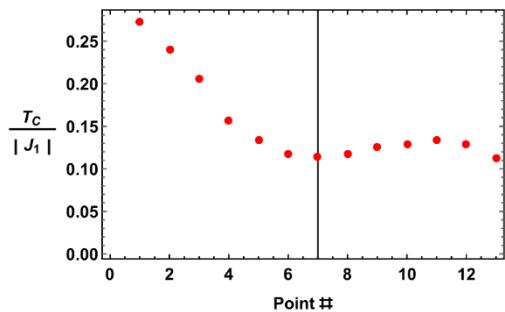


- 1) P. Chandra, P. Coleman, A.I. Larkin et al. Phys. Rev. Lett. **64**, 88 (1990)
- 2) L. Capriotti and S. Sachdev, Phys. Rev. Lett. **93**, 257206 (2004)
- 3) L. Seabra et al., Phys. Rev. B **93**, 085132 (2016)



Finite-temperature Z_2 (Ising) transition (Monte-Carlo)

Critical temperatures:



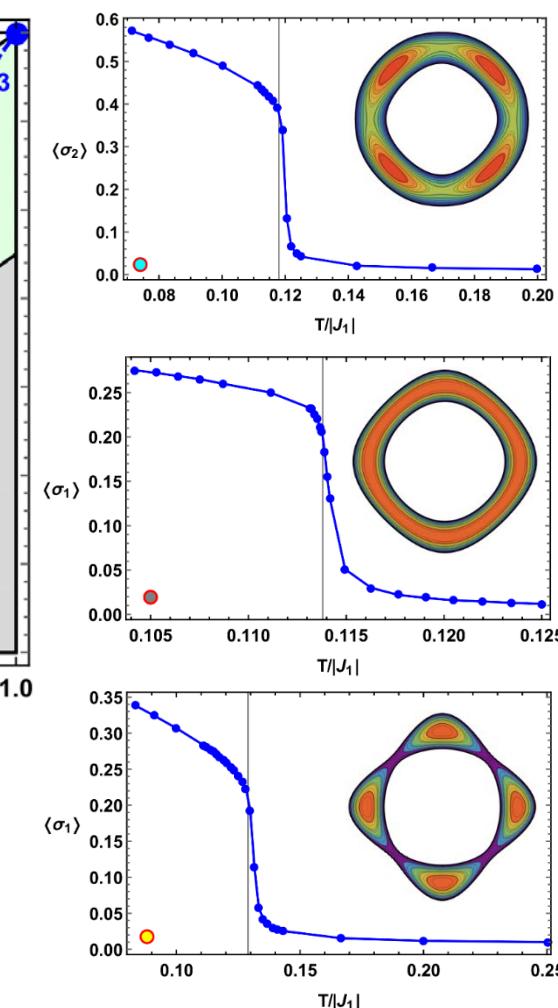
C_4 -breaking order-parameters:

Diagram illustrating the calculation of σ_1 . A central red dot r_i has two green dots at $(0, a)$ and two red dots at $(a, 0)$. A dashed green line connects the top green dot to the right red dot. A dashed red line connects the left red dot to the bottom green dot.

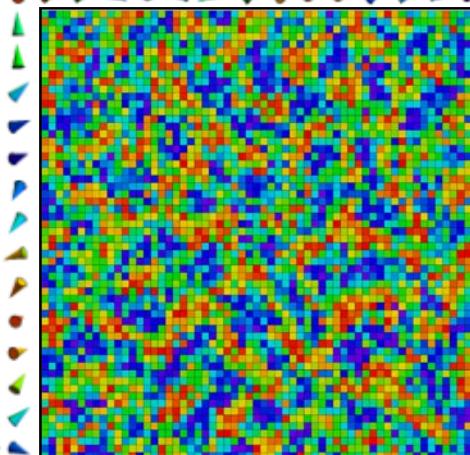
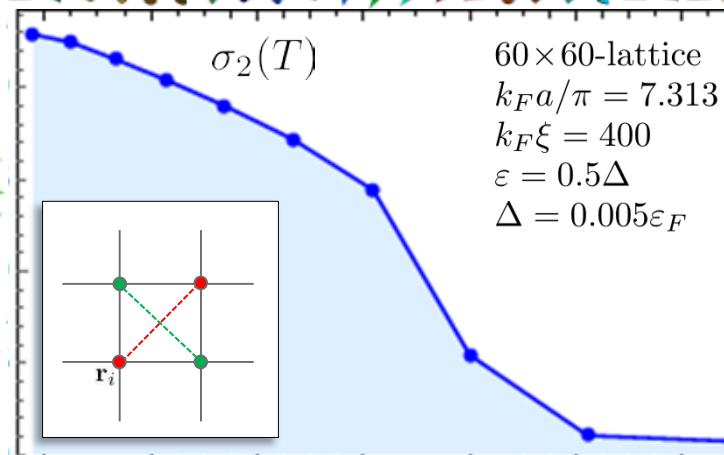
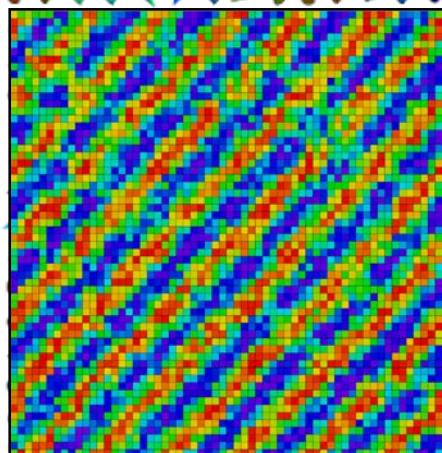
$$\sigma_1 = \frac{1}{N} \sum_i \left(\vec{S}_{\mathbf{r}_i} \cdot \vec{S}_{\mathbf{r}_i + (0, a)} - \vec{S}_{\mathbf{r}_i} \cdot \vec{S}_{\mathbf{r}_i + (a, 0)} \right)$$

Diagram illustrating the calculation of σ_2 . A central red dot r_i has four green dots at $(0, a)$, $(a, 0)$, $(0, -a)$, and $(-a, 0)$. A dashed green line connects the top green dot to the right red dot. A dashed red line connects the left red dot to the bottom green dot.

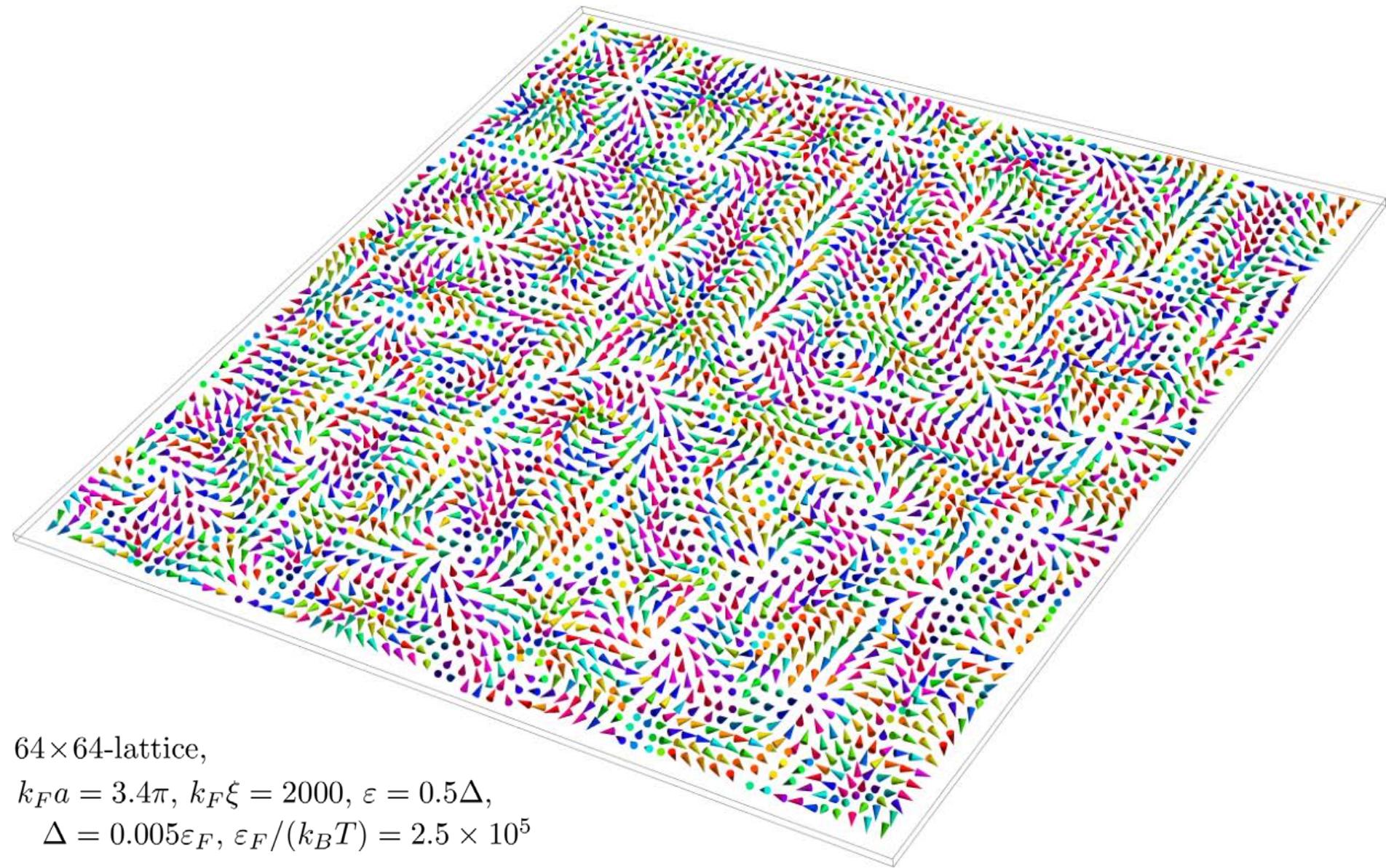
$$\sigma_2 = \frac{1}{N} \sum_i \left(\vec{S}_{\mathbf{r}_i} \cdot \vec{S}_{\mathbf{r}_i + (a, a)} - \vec{S}_{\mathbf{r}_i + (0, a)} \cdot \vec{S}_{\mathbf{r}_i + (a, 0)} \right)$$



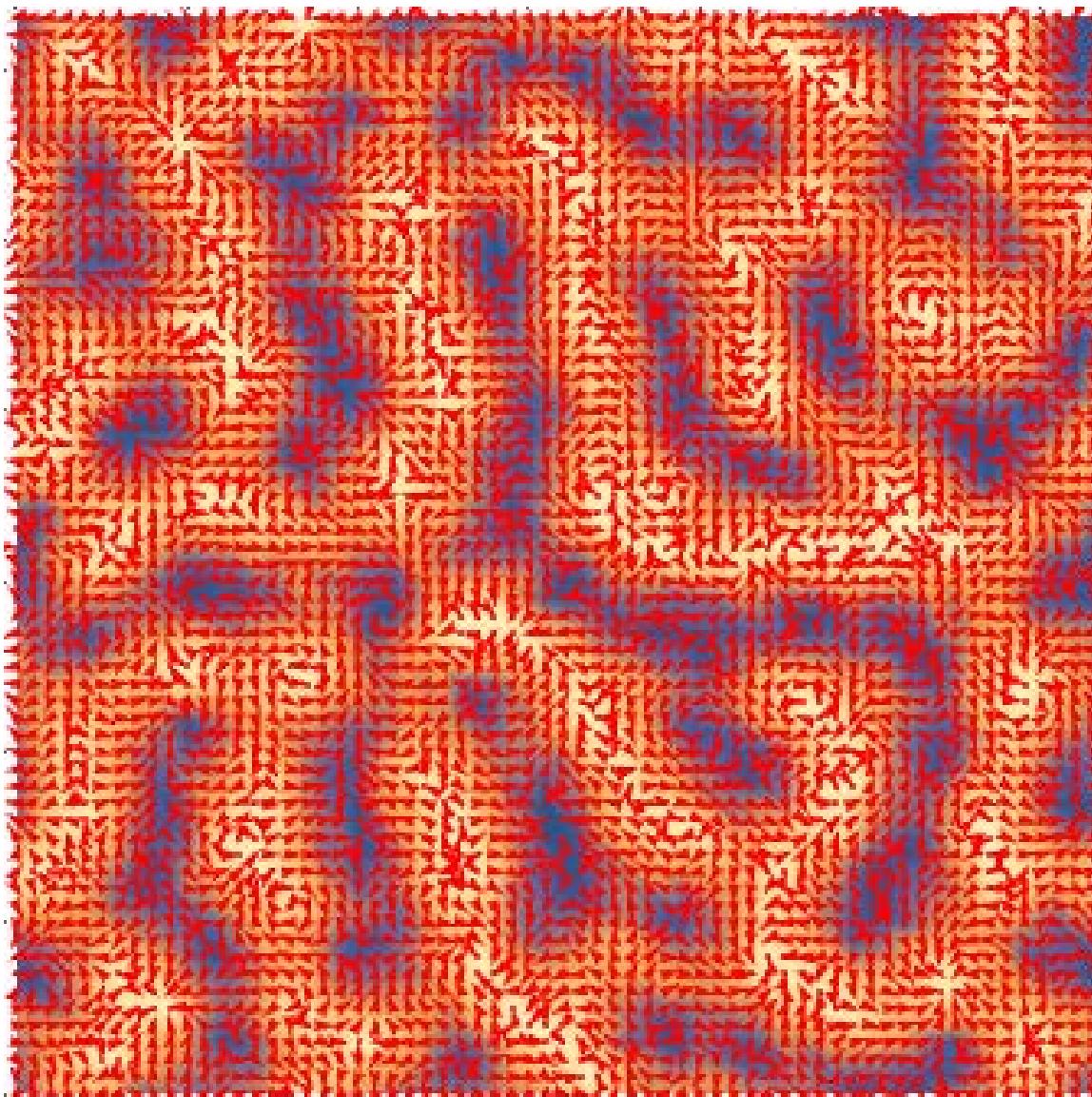
Finite-temperature Z_2 (Ising?) transition (**BCS+YSR**) (Monte-Carlo)



Frustrated spin configuration (**BCS+YSR**) (Monte-Carlo)

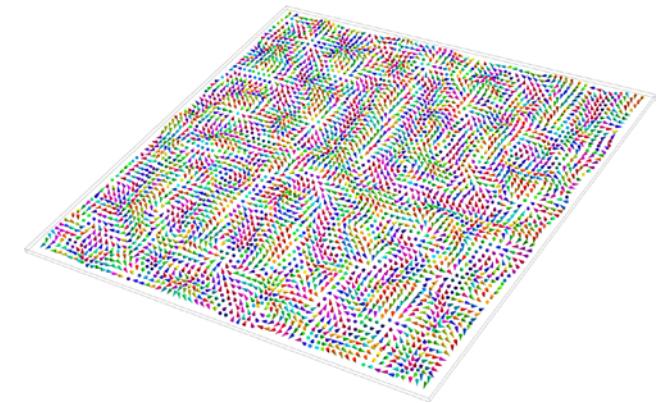


Frustrated spin configuration (**BCS+YSR**) (Monte-Carlo)



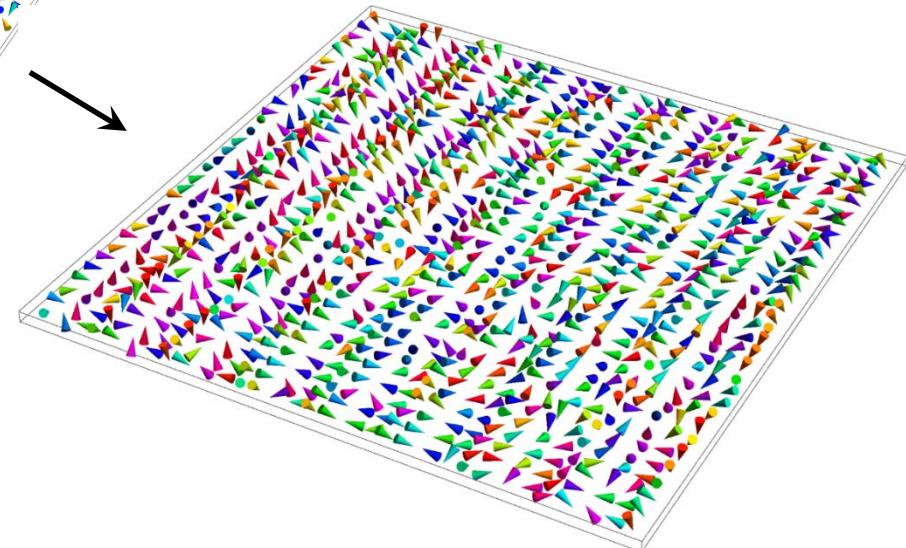
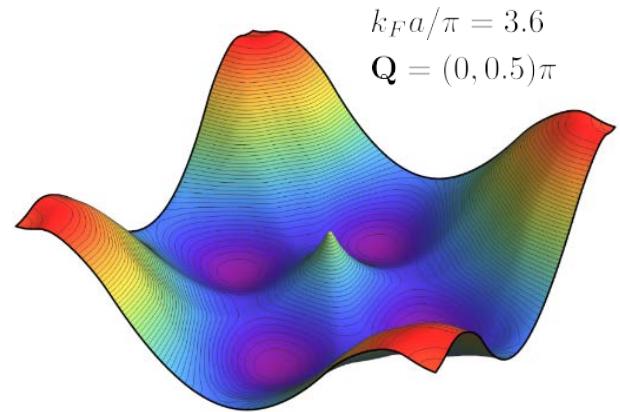
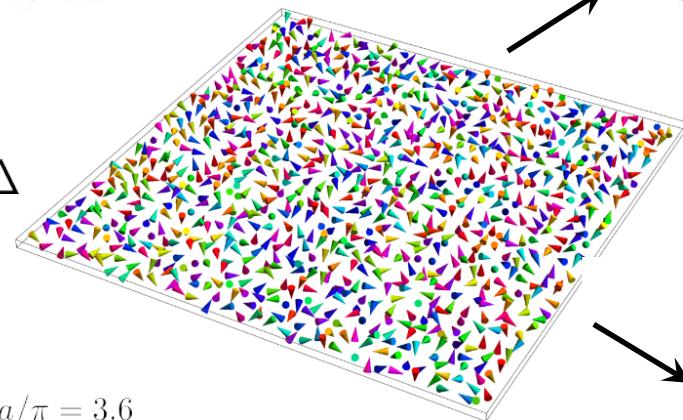
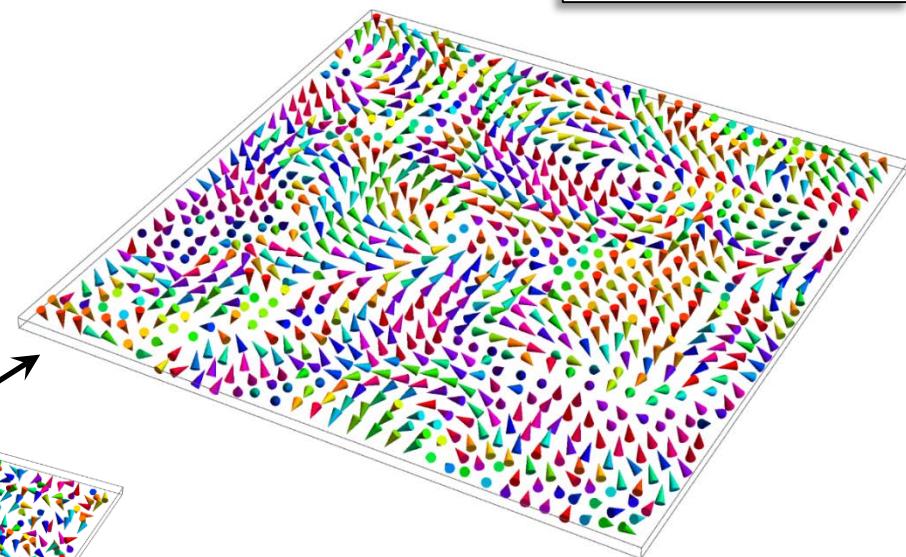
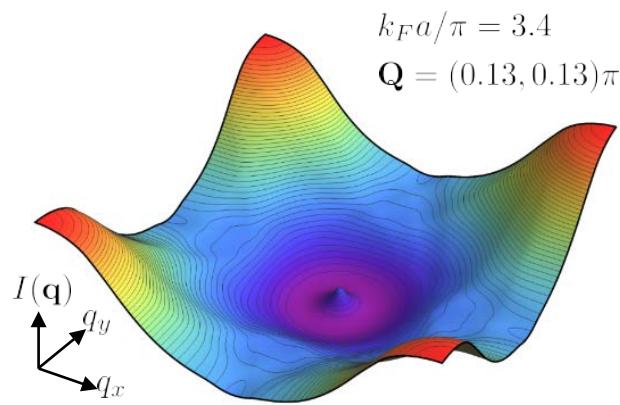
Z-axis projection (density)

XY-projection (red arrows)

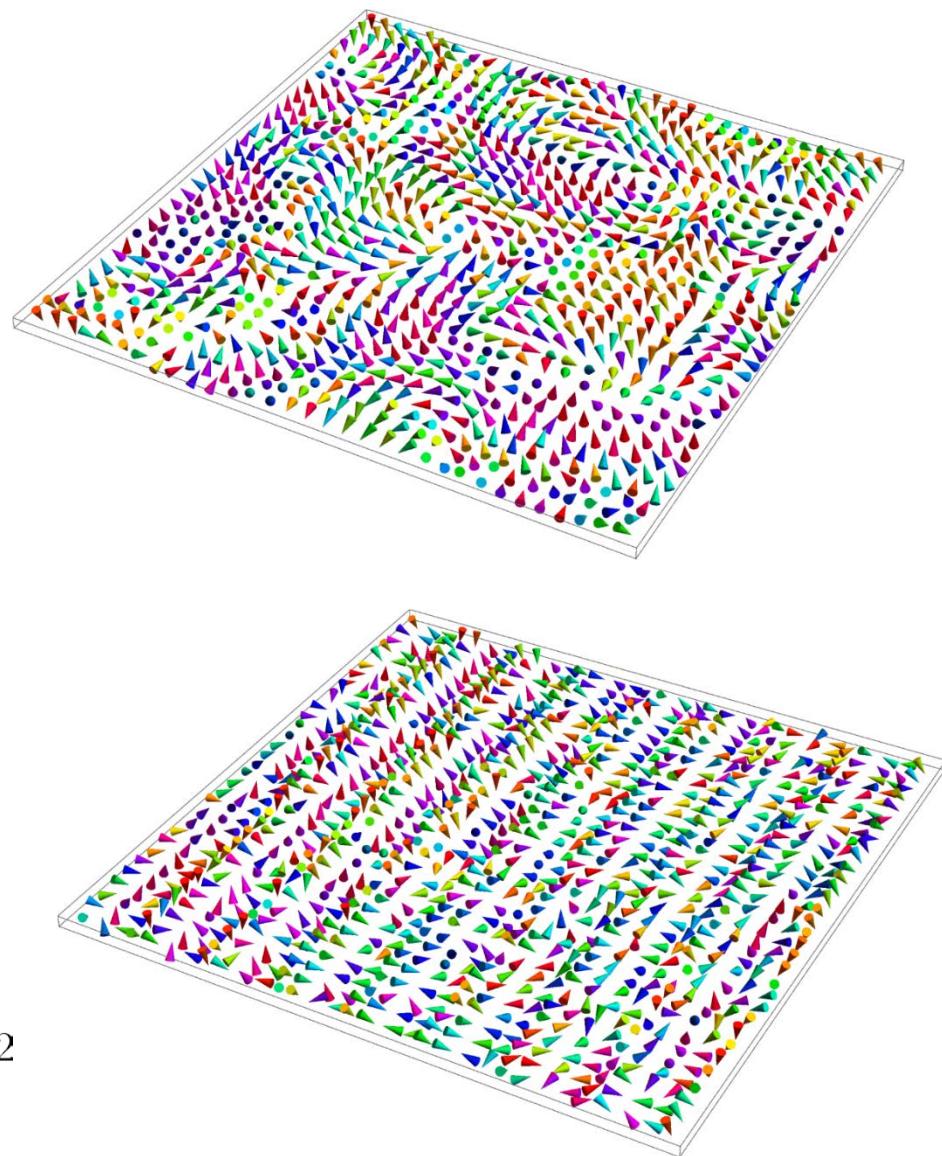
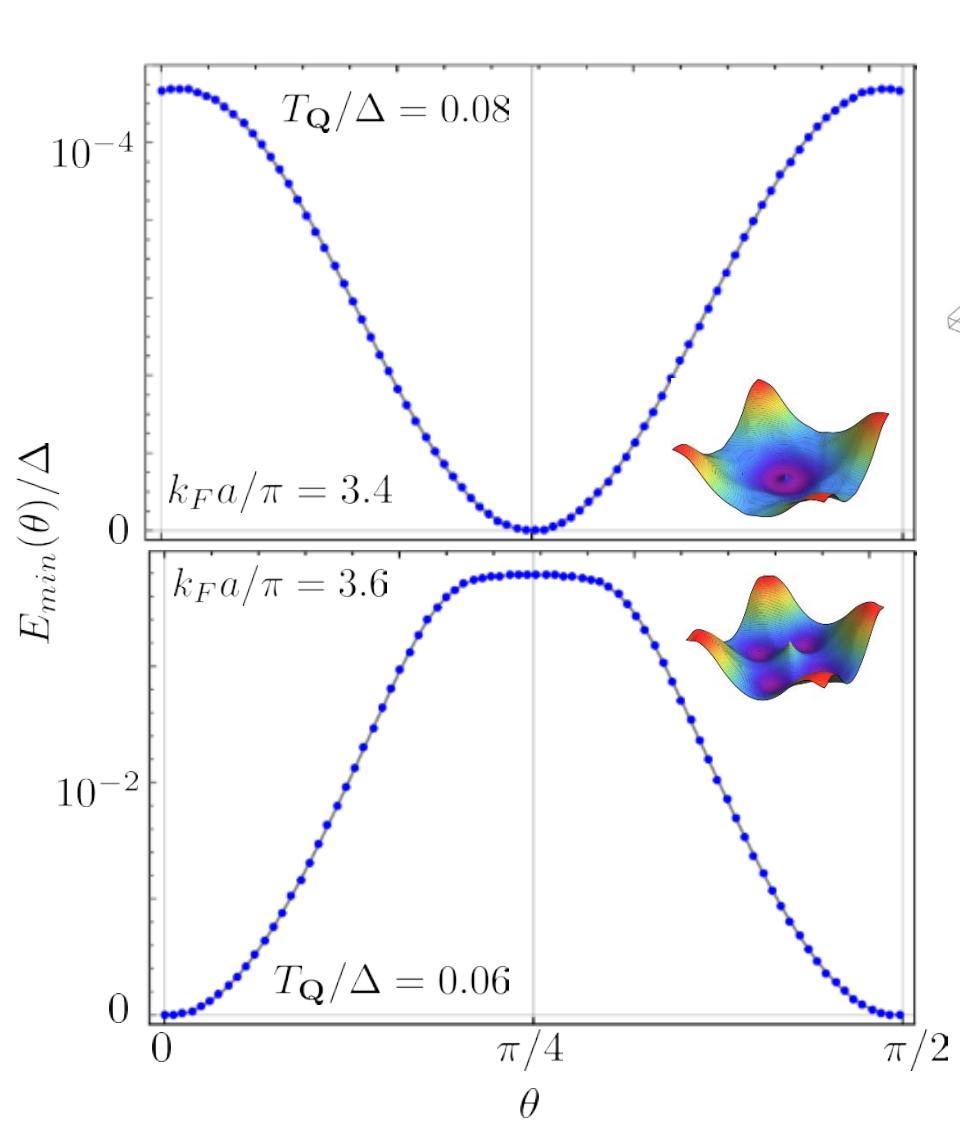


Energy-landscapes and spin configurations (BCS+YSR)

$\Delta = 0.005E_F$
 $k_F\xi = 400, \varepsilon = 0.5\Delta$

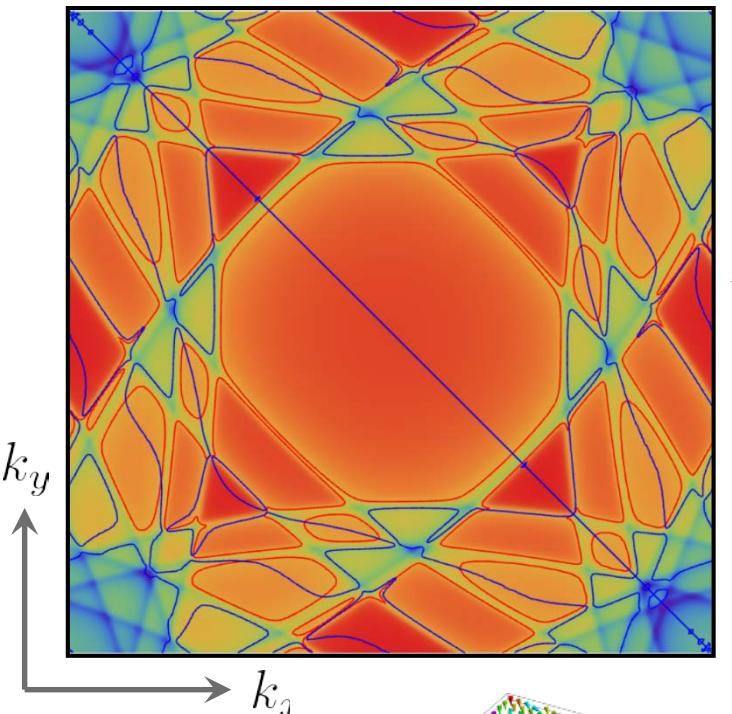


Angular energy barriers at radial minima: Frustration

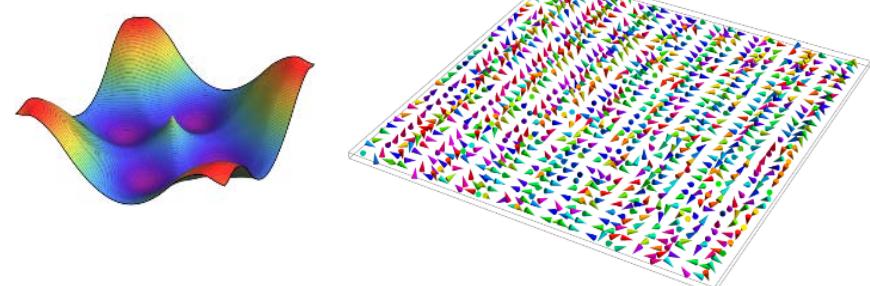
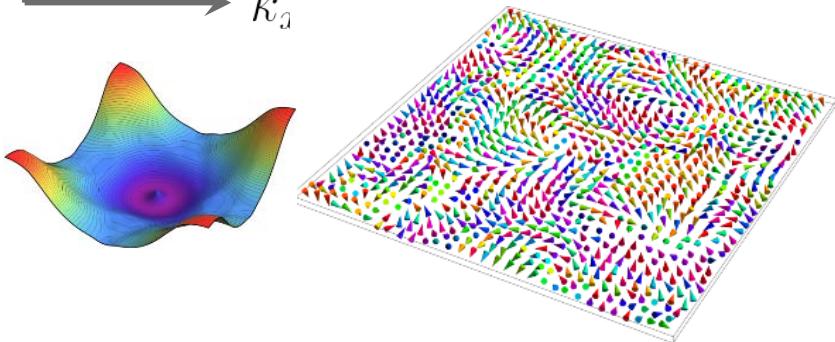
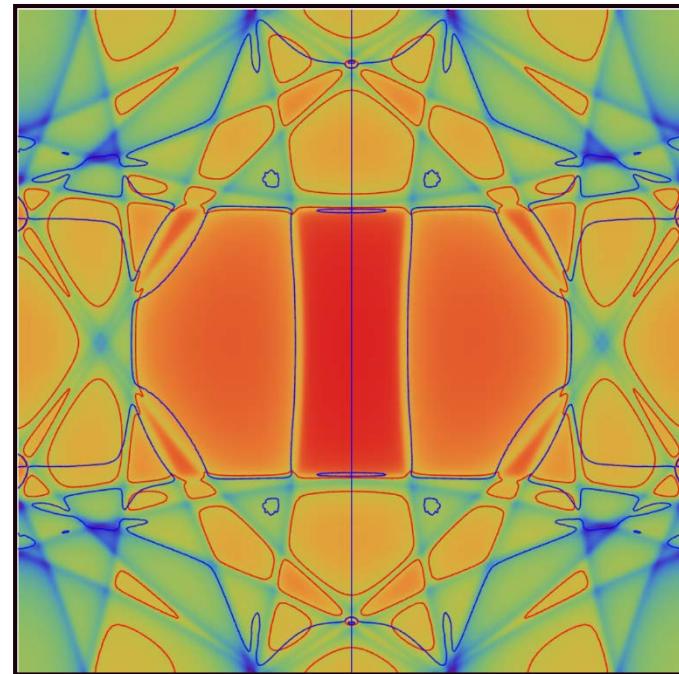


YSR sub-gap band-structure

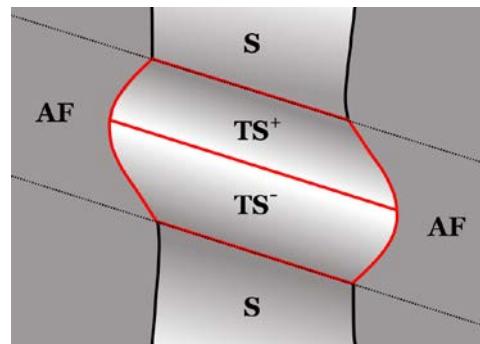
$$k_F a/\pi = 3.4 \quad \mathbf{Q} = (0.13, 0.13)\pi$$



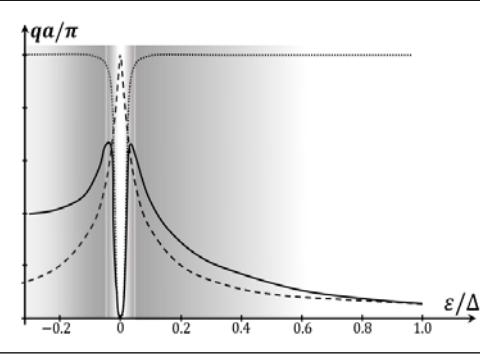
$$k_F a/\pi = 3.6 \quad \mathbf{Q} = (0, 0.5)\pi$$



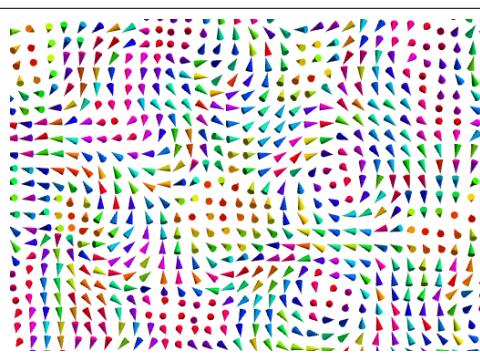
Summary & outlook



- Ferromagnetism destabilized by SC
- Even more so with YSR bound states
- Self-organized p-wave SC with Majoranas



- Deep YSR states give high-pitch spiral...
- ...but very deep YSR can give FM
- Double-exchange vs. Cooper-pair tunneling



- SC provides frustrated long-ranged exch.
- Rich magnetism for 2D in 3D SC...
- Multiple sub-gap top-band crossings...