

Coherent long range magnetic bound states in two-dimensional superconductors

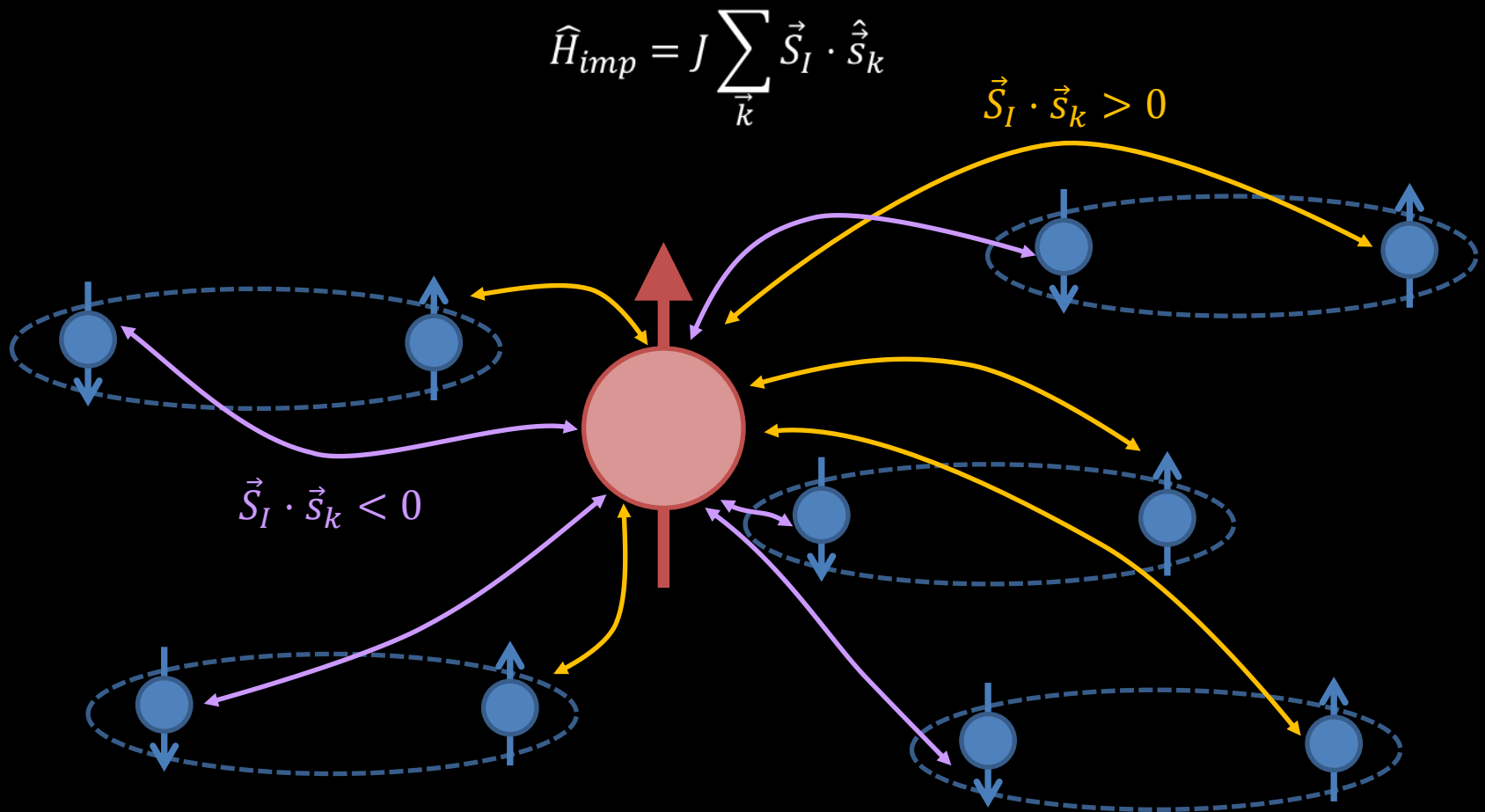
Tristan Cren

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CNRS & UPMC@Sorbonne University



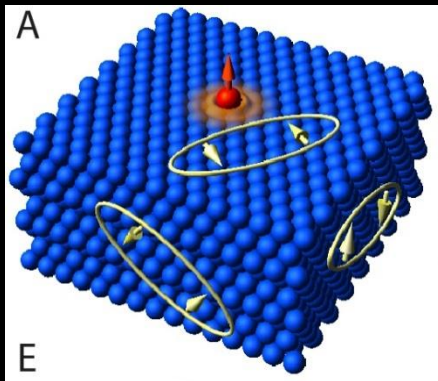
Classical magnetic impurities in a superconductor

Classical impurity approximation: the impurity behaves as a local magnetic field

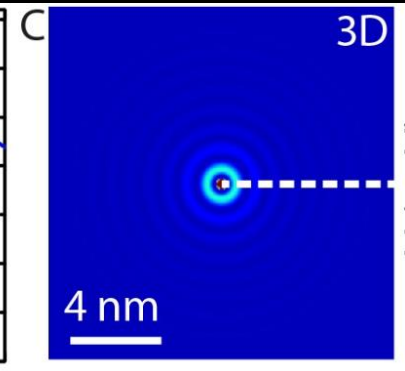
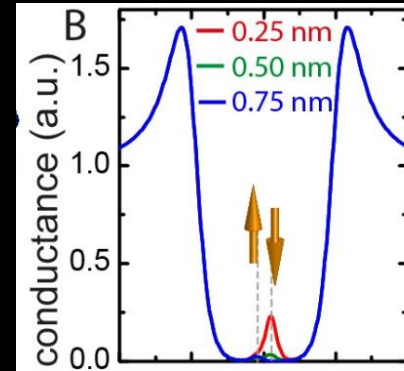


Magnetic impurities: Interaction mechanism

Appearance of in-gap Yu-Shiba-Rusinov bound states localized around the magnetic impurity



$$\hat{H}_{imp} = J \sum_{\vec{k}} \vec{S}_I \cdot \hat{S}_{\vec{k}}$$



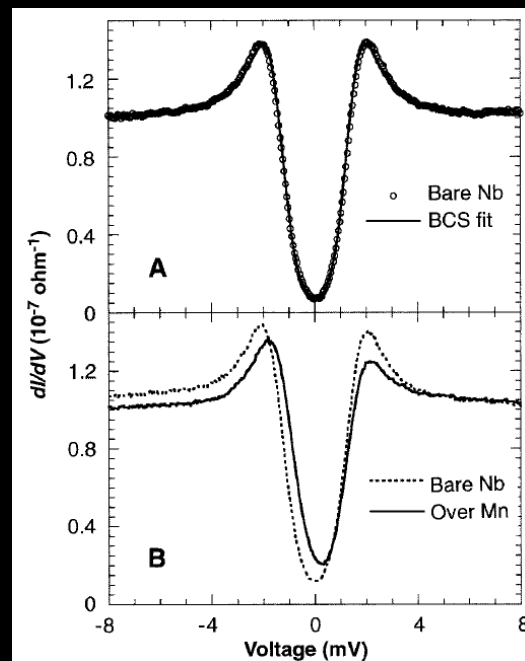
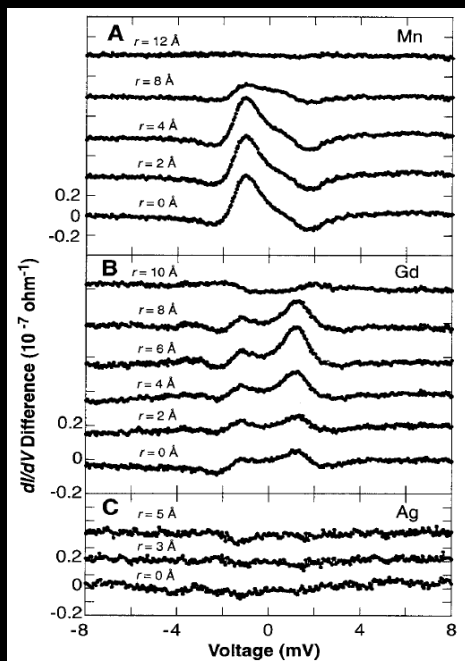
$$\psi_{\pm}(r) = \frac{1}{\sqrt{N}} \frac{\sin(k_F r + \delta^{\pm})}{k_F r} e^{-\Delta \sin(\delta^+ - \delta^-) r / \hbar v_F}$$

$$E = \Delta \cos(\delta^+ - \delta^-)$$

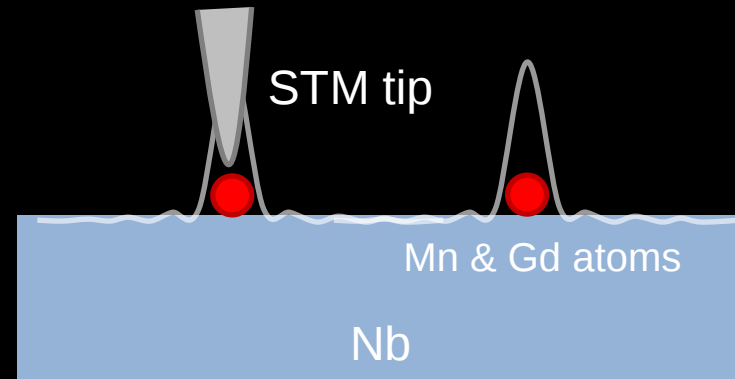
$$\tan \delta^{\pm} = (K \nu_0 \pm \nu_0 J S / 2)$$

Single magnetic impurities observed by STM

- Bound states for magnetic impurities (Mn & Gd) on Nb
- No bound states for non magnetic Ag adatoms on Nb



Yazdani et al. *Science* **275**, 1767 (1997)



The wave function of the bound states is localized at less than 10 Å from the impurities

Single magnetic impurities observed by STM

Angular momentum

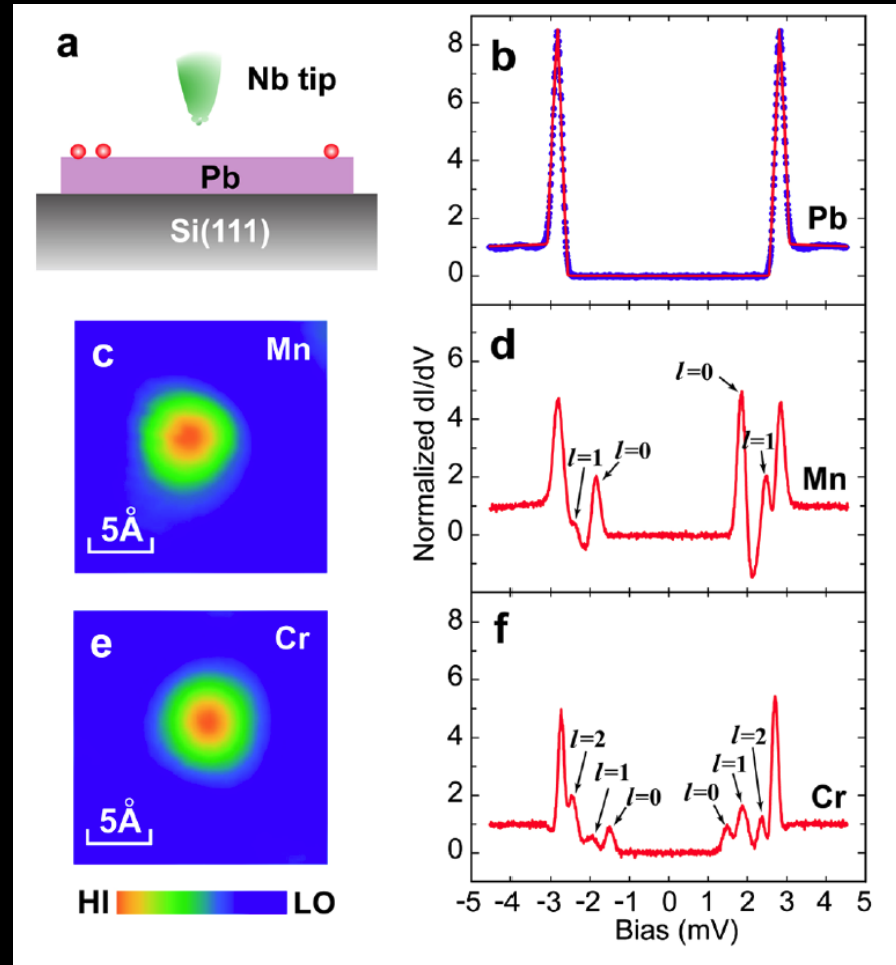
The number of Shiba peaks depends on the atom nature

$$\text{Mn} \rightarrow l = 0, 1$$

$$\text{Cr} \rightarrow l = 0, 1, 2$$

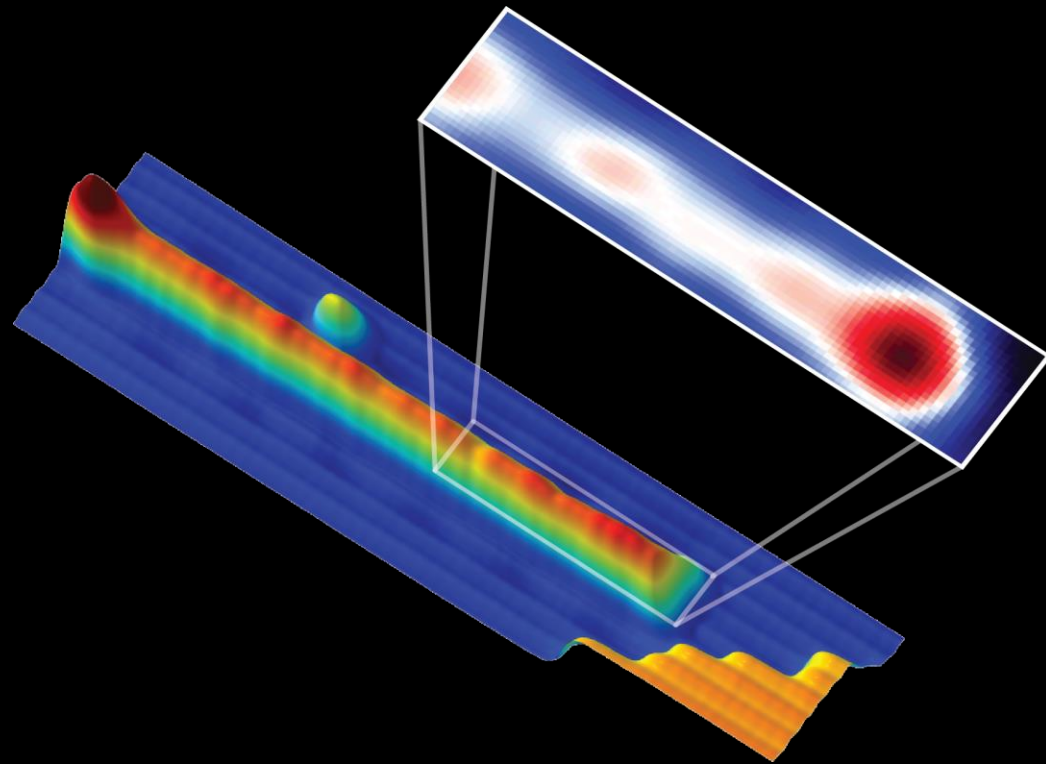
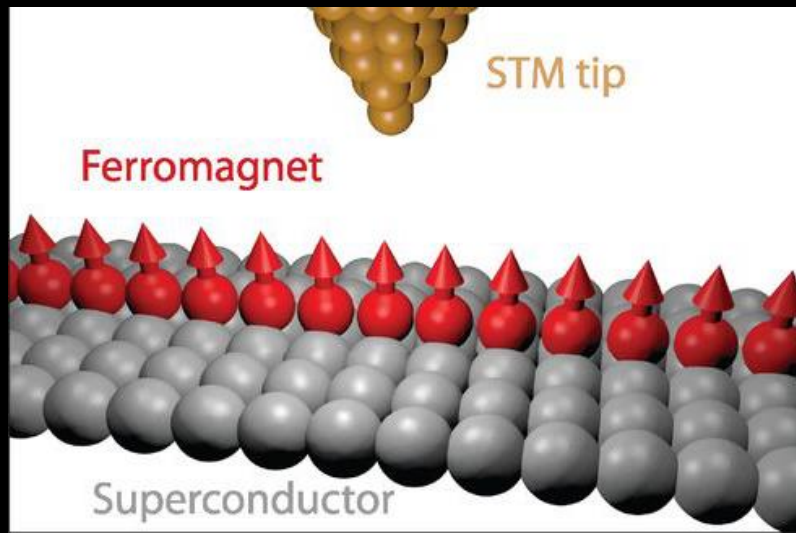
Every peak corresponds to a different diffusion channel for the superconducting electrons.

Extremely local effect of the impurities (a few Å)

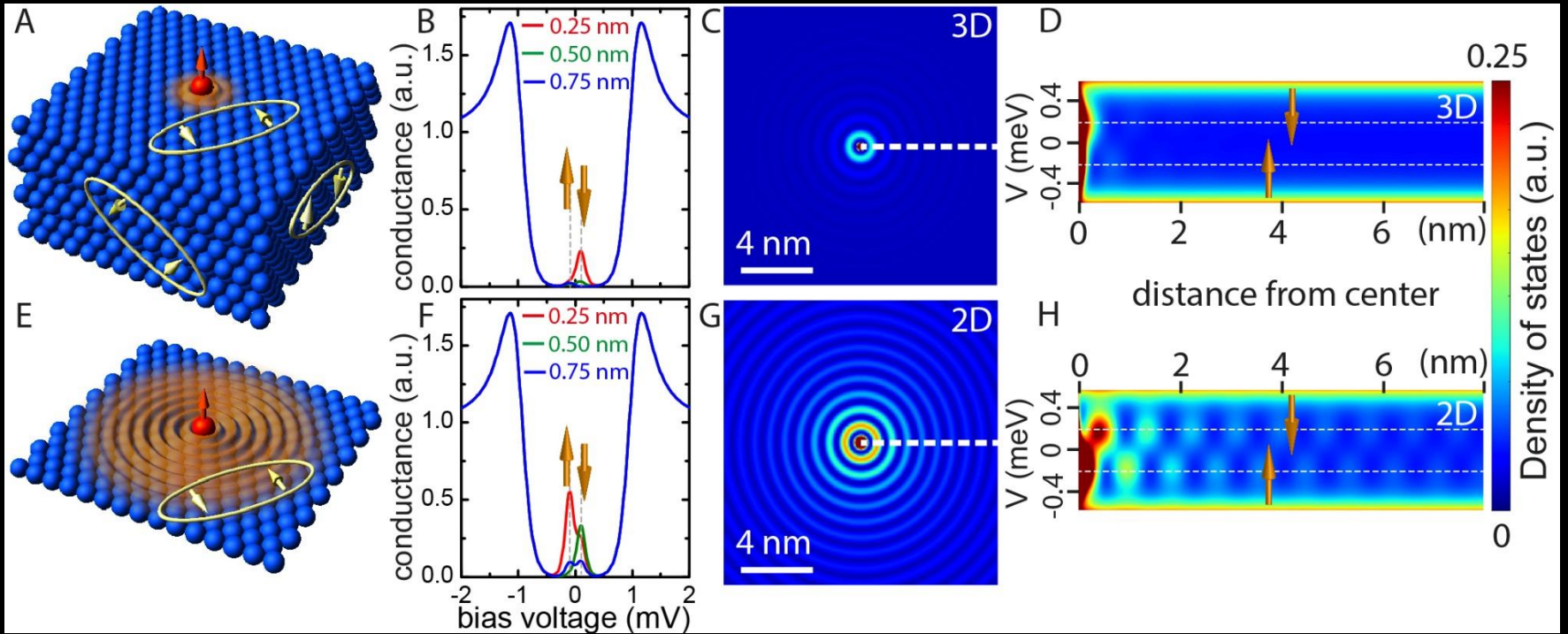


Majorana end states in magnetic chains : Fe/Pb(110)

Zero-bias anomaly localized on the last atoms of the Fe chain,
almost no extension into the Pb substrate



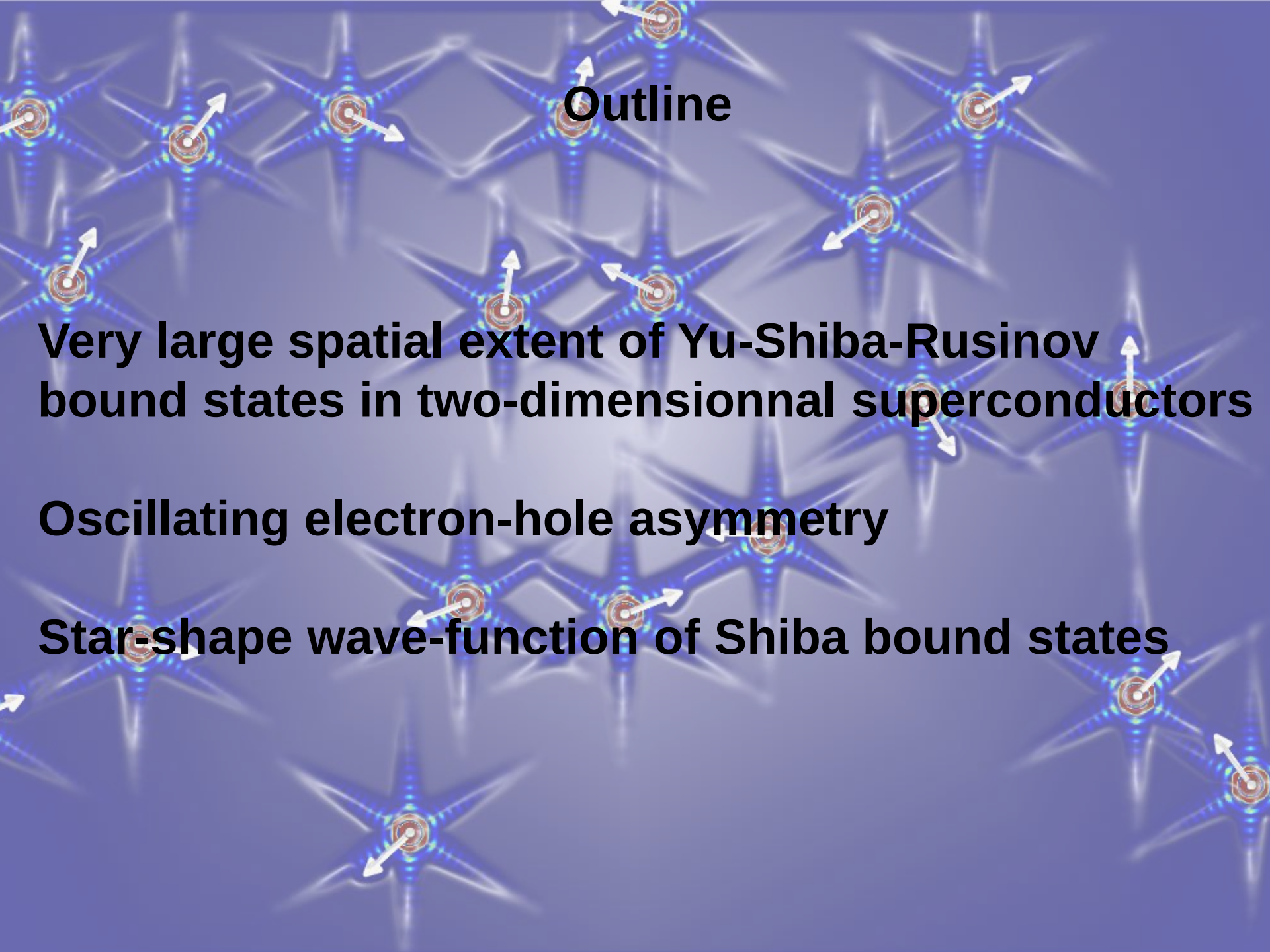
Spatial structure of the Yu-Shiba-Rusinov states 3D vs. 2D materials



At 3D : $1/r^2$ law for amplitude decrease of the density of states

At 2D : $1/r$ law for amplitude decrease of the density of states

$$\begin{aligned}
 \text{3D} &\longrightarrow \psi_{\pm}(r) = \frac{1}{\sqrt{N}} \frac{\sin(k_F r + \delta^{\pm})}{k_F r} e^{-\Delta \sin(\delta^+ - \delta^-) r / \hbar v_F} \\
 \text{2D} &\longrightarrow \psi_{\pm}(r) = \frac{1}{\sqrt{N \pi k_F r}} \sin(k_F r - \frac{\pi}{4} + \delta^{\pm}) e^{-\Delta \sin(\delta^+ - \delta^-) r / \hbar v_F}
 \end{aligned}$$



Outline

Very large spatial extent of Yu-Shiba-Rusinov bound states in two-dimensionnal superconductors

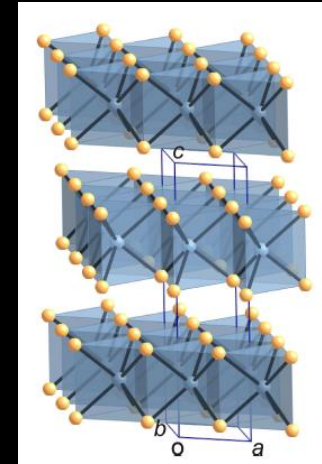
Oscillating electron-hole asymmetry

Star-shape wave-function of Shiba bound states

Two-dimensional superconductors

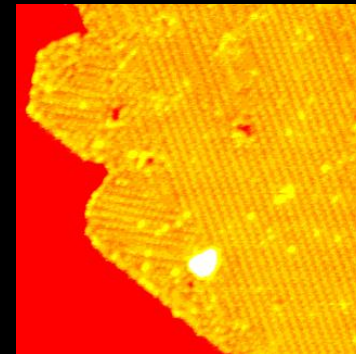
- Bulk superconductor with 2D electronic structure:

Lamellar material 2H-NbSe_2

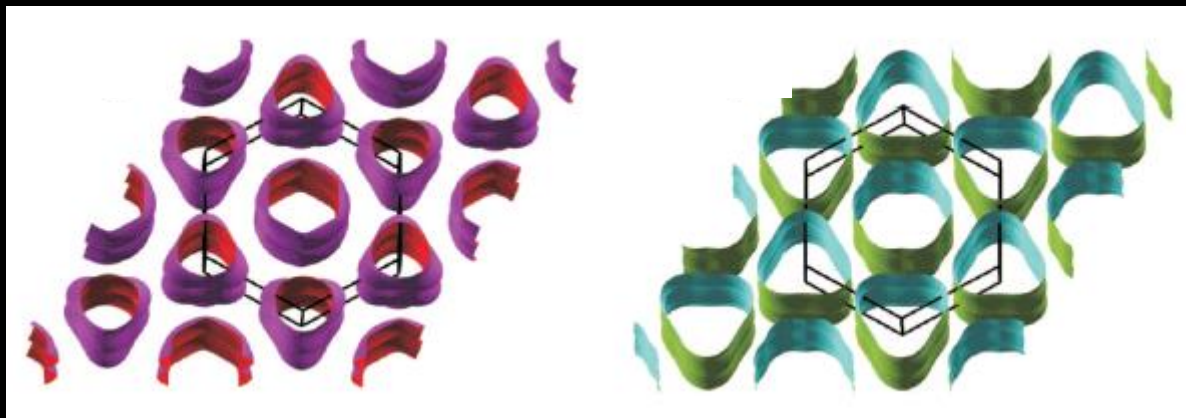
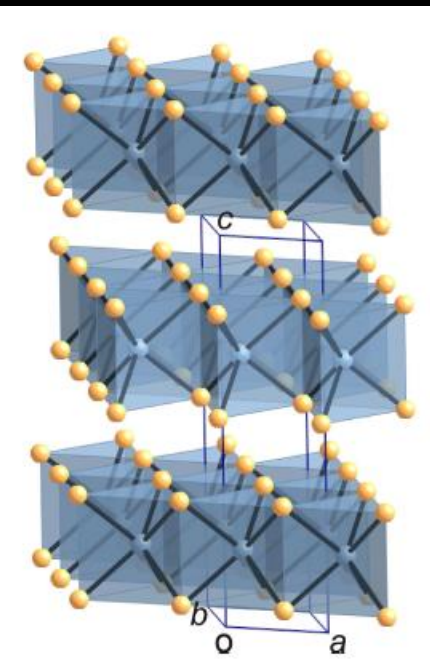


- Ultimately thin superconductor :

Single atomic layer of Pb/Si(111)



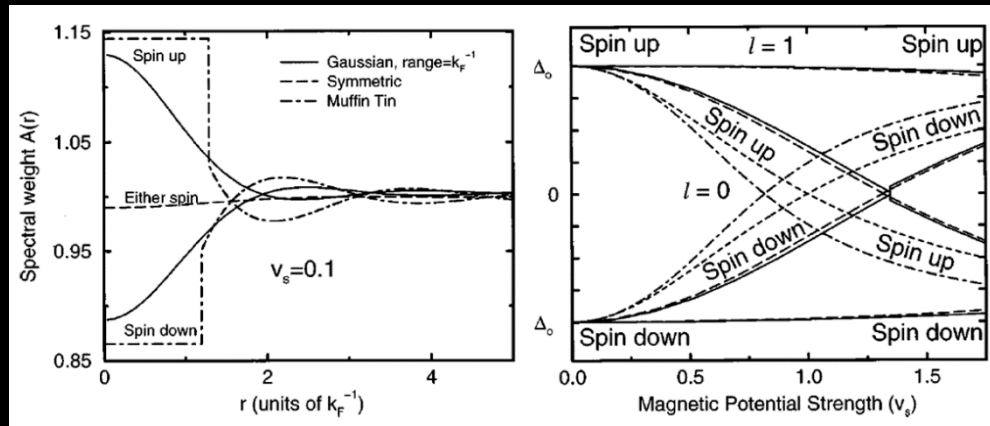
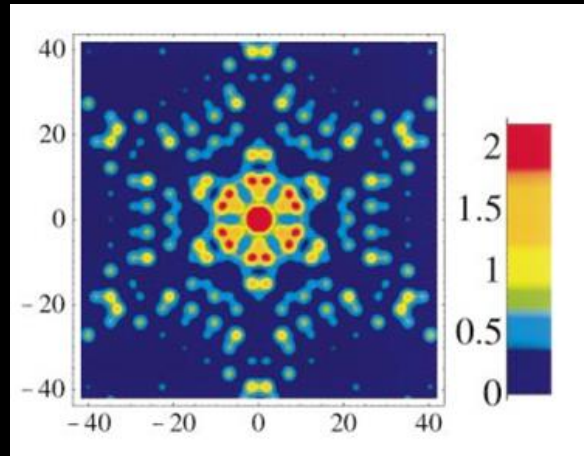
2H-NbSe₂ as a two-dimensional superconductor



Two-dimensional like bands structure due to the weak Van der Waals interlayer coupling.

Magnetic impurities in 2H-NbSe₂

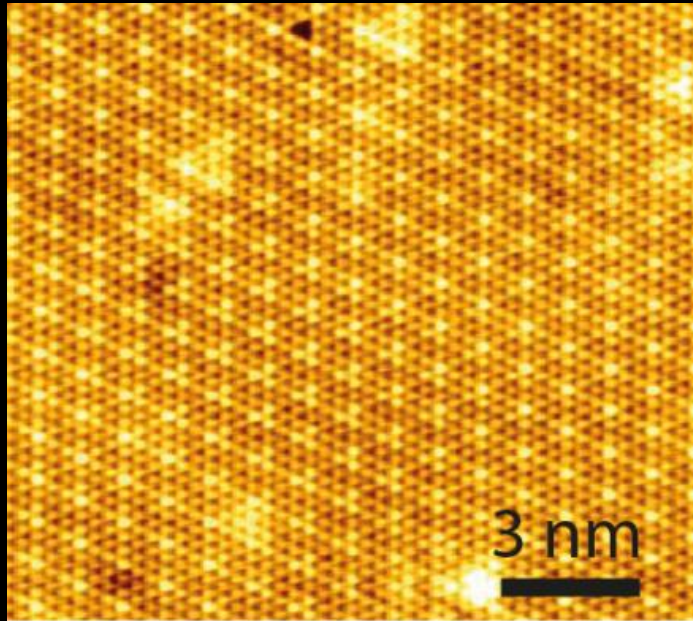
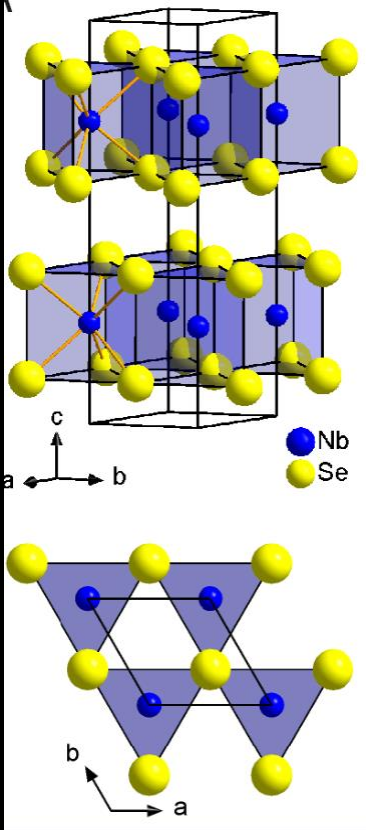
Prediction of a star shape Yu-Shiba-Rusanov bound state



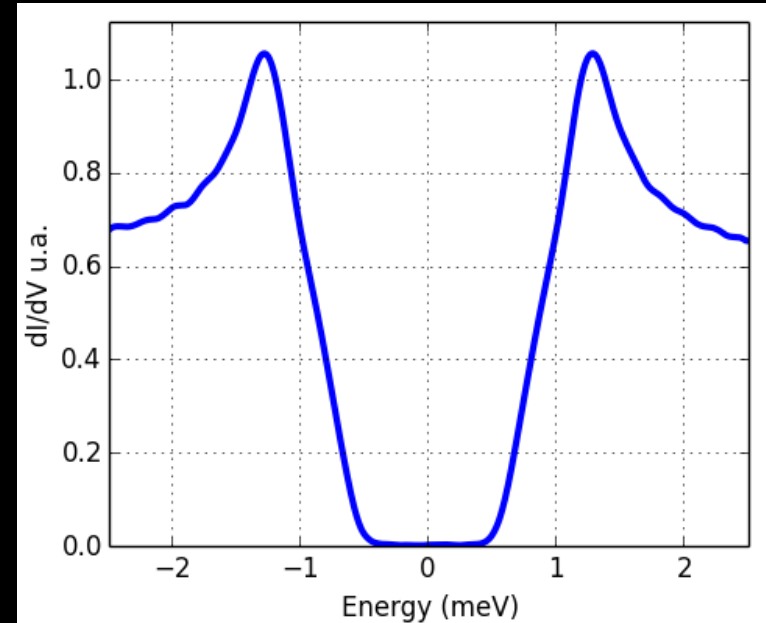
M.E. Flatté and J.M. Byers. *PRL* **78**, 3761 (1997)

A classical spin in 2H-NbSe₂ may give rise to a bound state with a star shaped pattern

2H-NbSe₂ as a two-dimensional superconductor

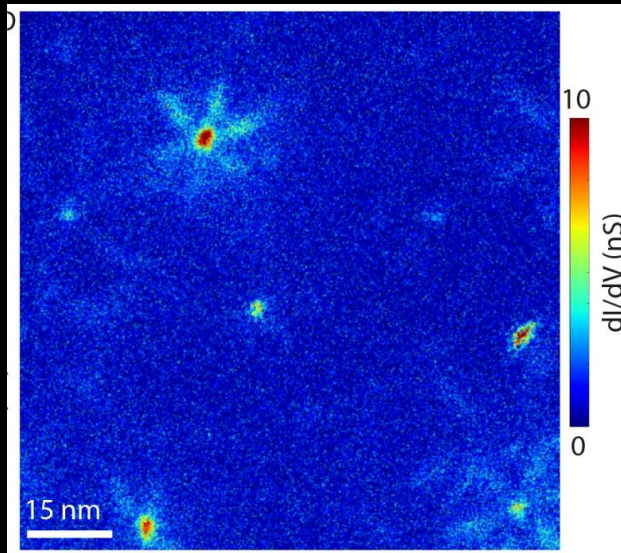


Topography
Atomic lattice and 3x3 CDW



Superconducting gap
measured at 320 mK
(multigap superconductor)

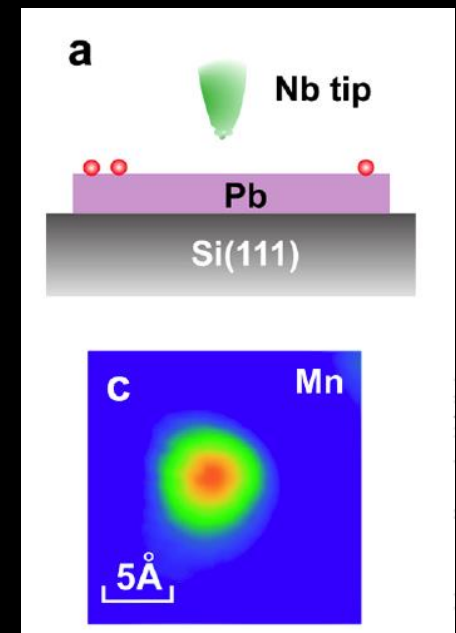
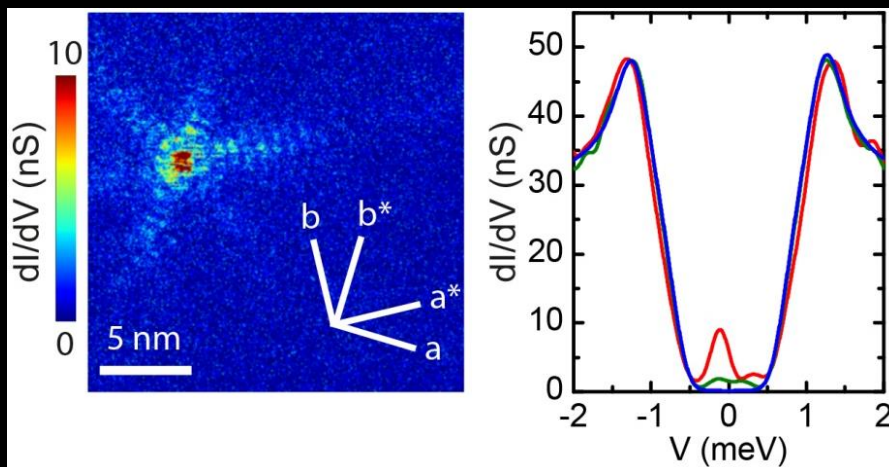
Observation of bound states around magnetic impurities in 2H-NbSe₂



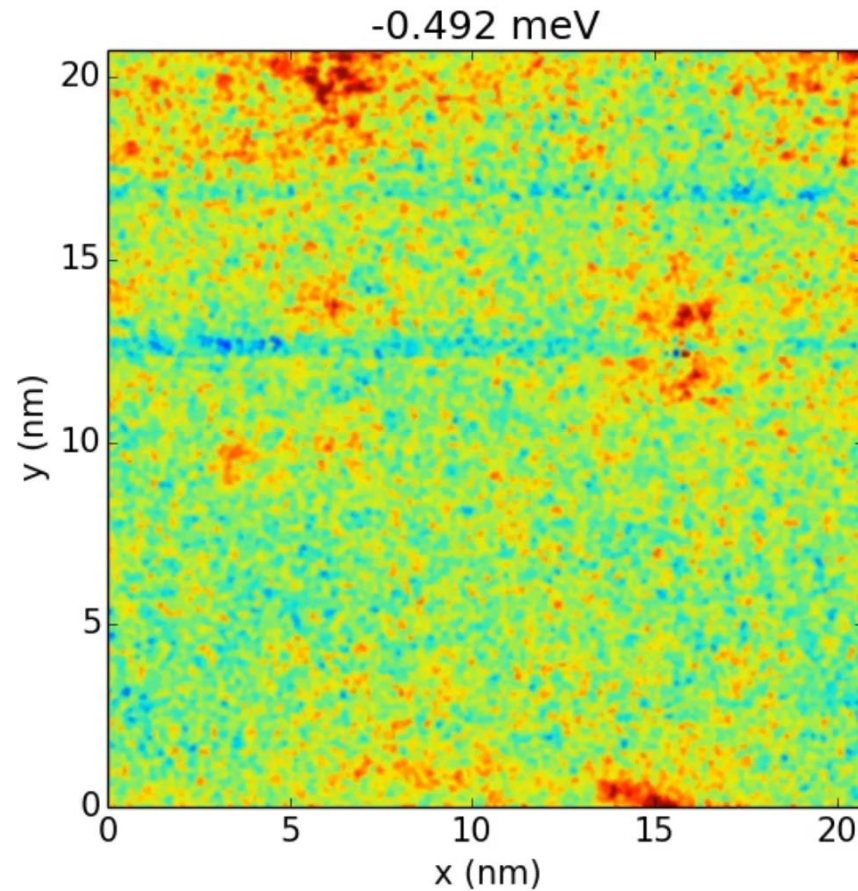
The Nb used for the crystal growth contains magnetic impurities :

- 175 ppm of Fe
- 54 ppm of Cr
- 22 ppm of Mn

dI/dV maps at -0.13 mV (320 mK)

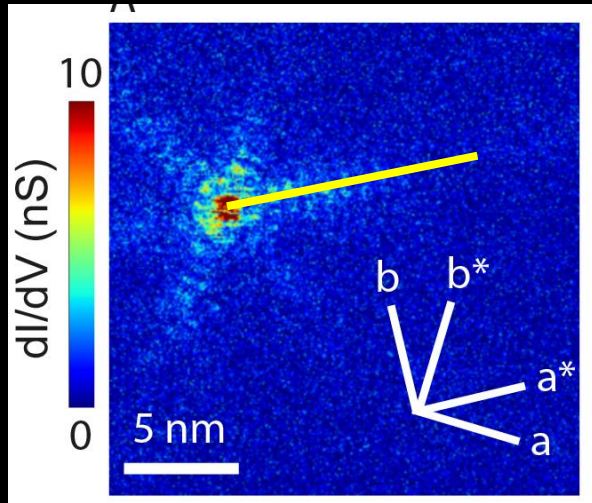


Observation of bound states around magnetic impurities in 2H-NbSe₂

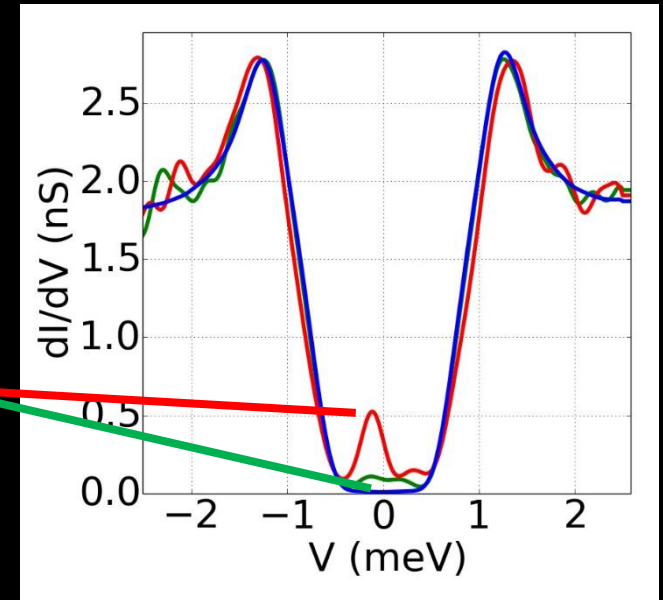
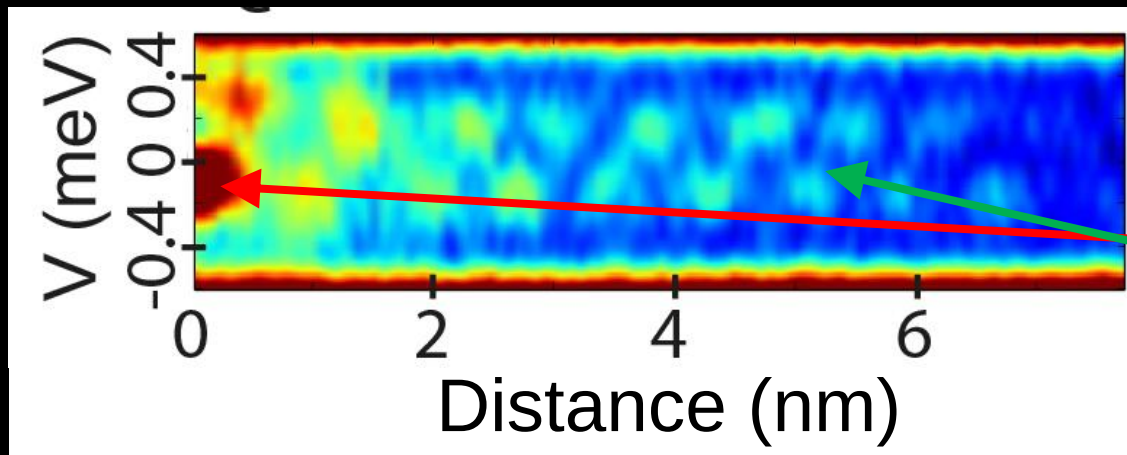


Spatial oscillation of Shiba bound states

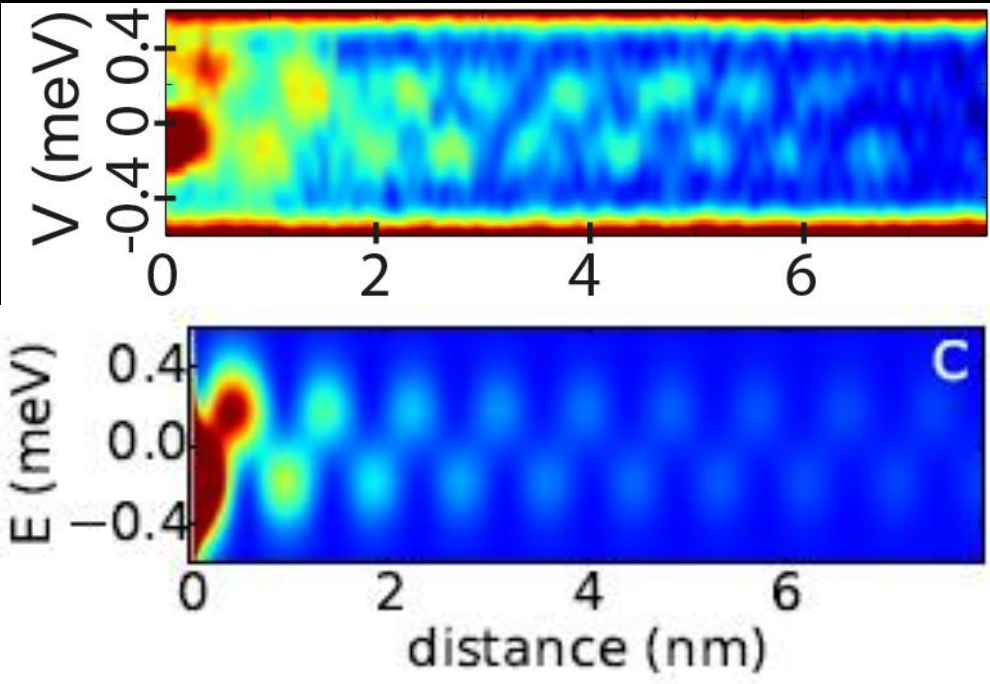
Electron-hole asymmetry



- Oscillations of the local density of states with a phase opposition between positive and negative energy states
- Decrease of the Shiba bound states on a size of the order of the coherence length ξ



Spatial oscillations and electron-hole asymmetry



Good agreement with theoretical calculations for 2D case in the asymptotic limit.

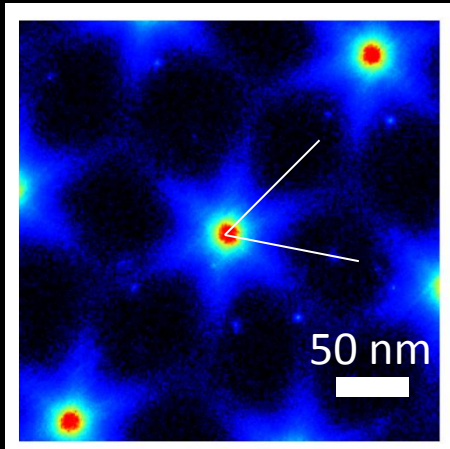
$$\psi_{\pm}(r) = \frac{1}{\sqrt{N\pi k_F r}} \sin\left(k_F r - \frac{\pi}{4} + \delta^{\pm}\right) e^{-\Delta \sin(\delta^+ - \delta^-) r / \hbar v_F}$$

$$E = \Delta \cos(\delta^+ - \delta^-)$$

$$\tan \delta^{\pm} = (K\nu_0 \pm \nu_0 JS/2)$$

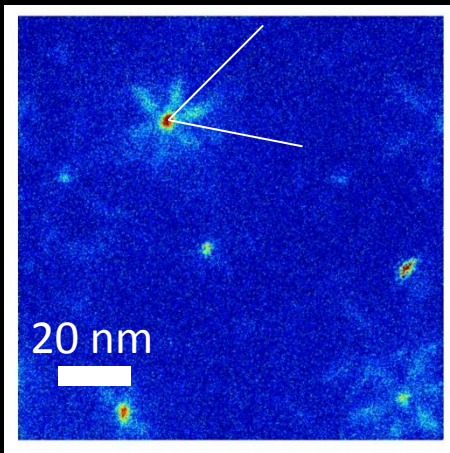
The Shiba peaks **position relatively to the gap** is directly related to the phase shift.

Six fold symmetry of the Shiba bound states



$H = 100\text{mT}$

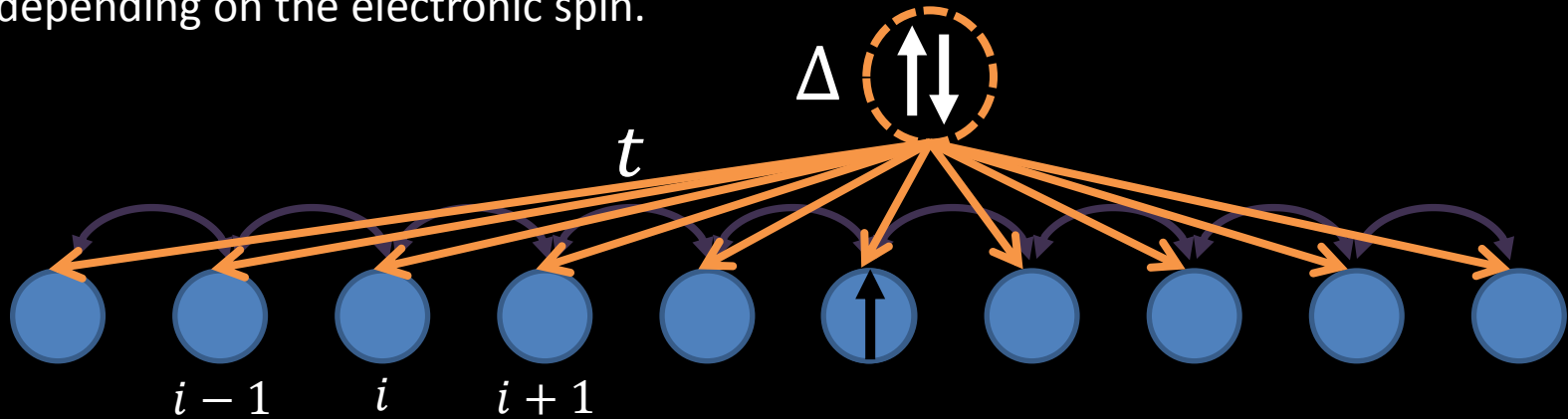
In NbSe₂ the star shape vortex cores are rotated 30° from the atomic lattice



The star shape structures of the magnetic bound states has the same orientation as the bound states in the vortex cores.

Theoretical model: Bogoliubov de Gennes

The magnetic interaction is modelled by an on-site energy term with a sign depending on the electronic spin.

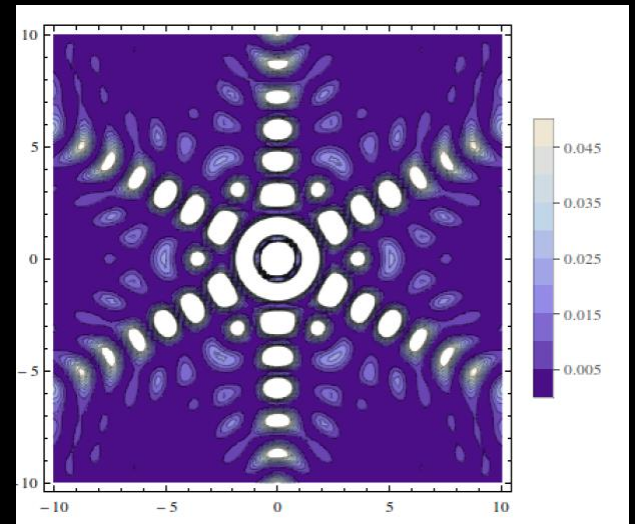
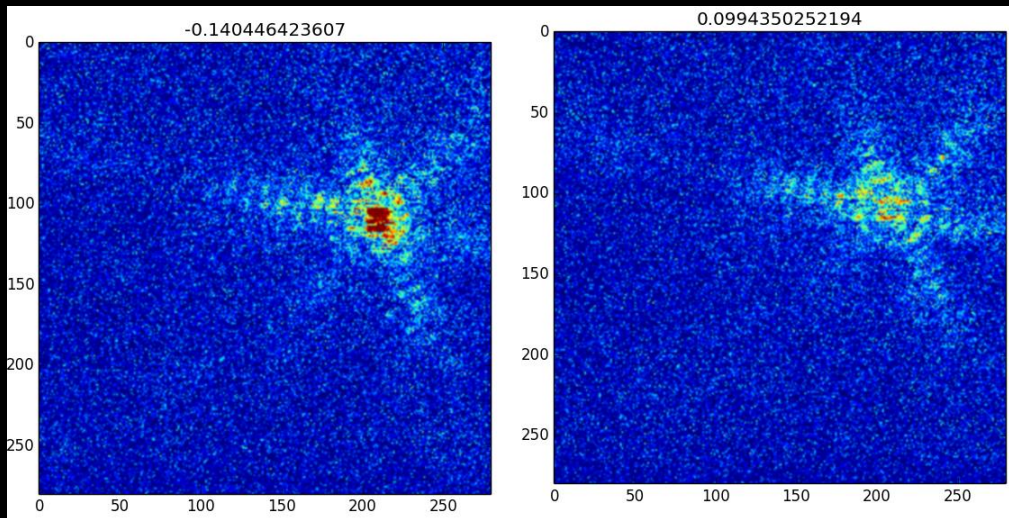


Hamiltonian expressed in the spinor basis $\psi = \begin{pmatrix} \psi_{\uparrow}^{\dagger} \\ \psi_{\downarrow} \\ \psi_{\downarrow}^{\dagger} \\ \psi_{\uparrow} \end{pmatrix}$

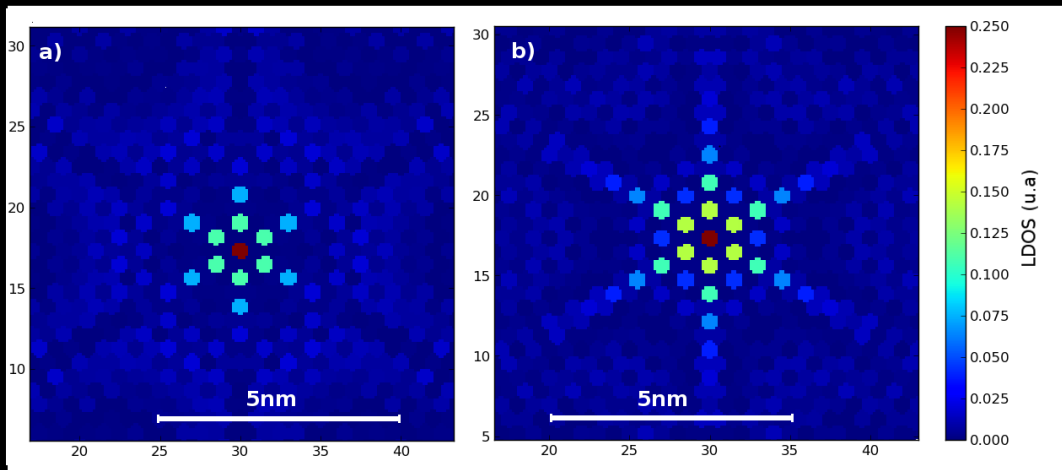
$$H_{BdG} = \sum_k \xi_k (\hat{c}_{k\uparrow}^{\dagger} \hat{c}_{k\uparrow} + \hat{c}_{k\downarrow}^{\dagger} \hat{c}_{k\downarrow}) + \Delta (\hat{c}_{k\uparrow}^{\dagger} \hat{c}_{k\downarrow}^{\dagger} + \hat{c}_{k\downarrow} \hat{c}_{k\uparrow})$$

$$H_{imp} = -\frac{JS}{2} (\hat{c}_{0\uparrow}^{\dagger} \hat{c}_{0\uparrow} - \hat{c}_{0\downarrow}^{\dagger} \hat{c}_{0\downarrow}) + K (\hat{c}_{0\uparrow}^{\dagger} \hat{c}_{0\uparrow} + \hat{c}_{0\downarrow}^{\dagger} \hat{c}_{0\downarrow})$$

Theoretical model: Bogoliubov de Gennes

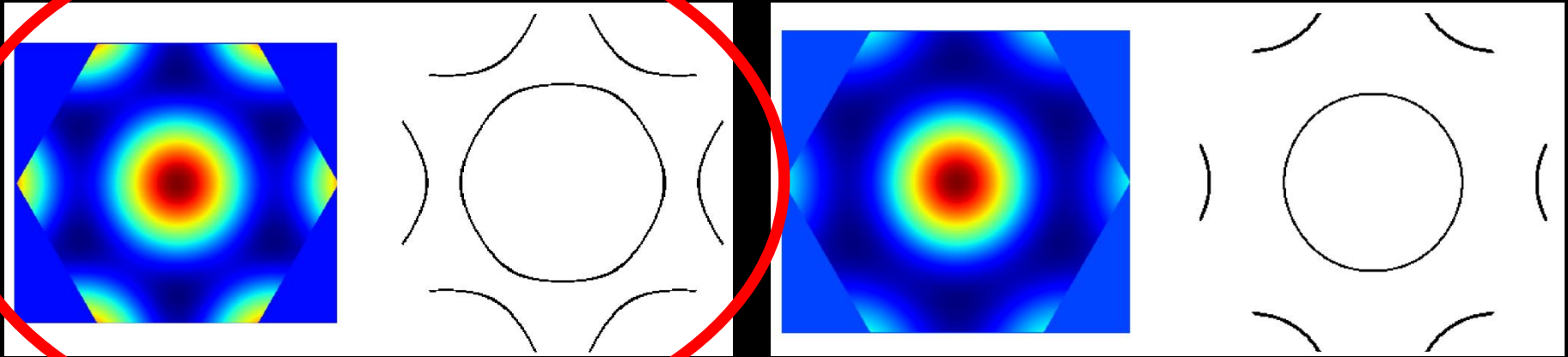


Continuous asymptotic model



Ongoing calculations using Wannier functions

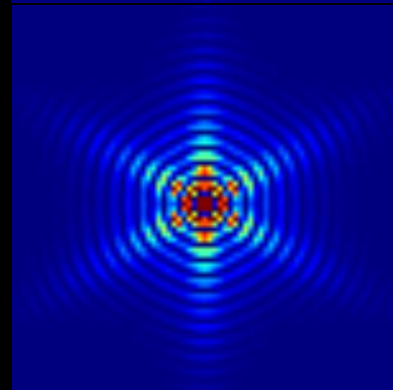
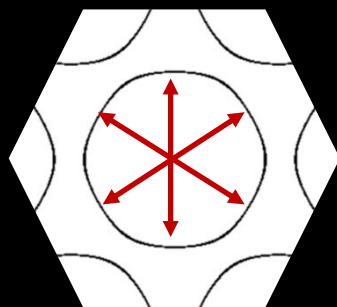
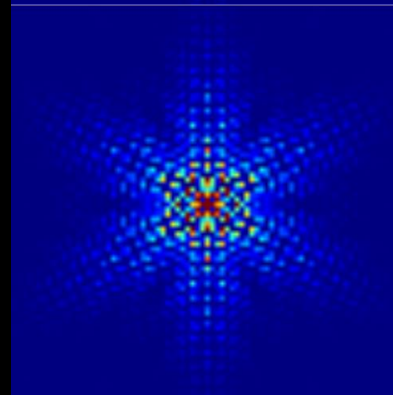
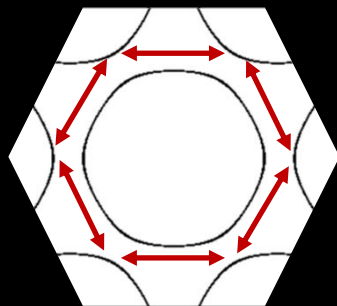
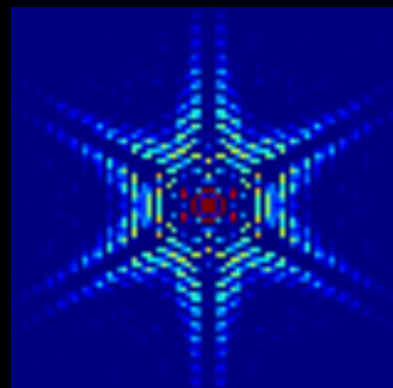
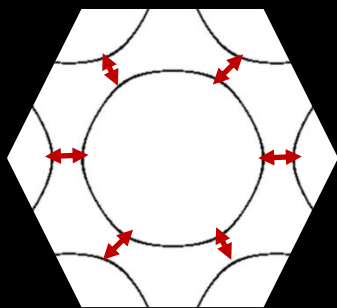
Six fold symmetry of the Bound states



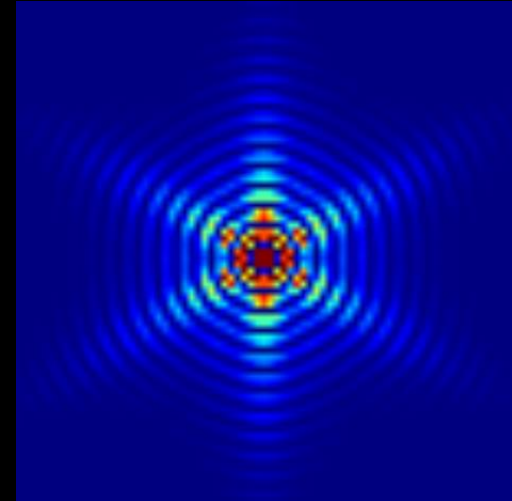
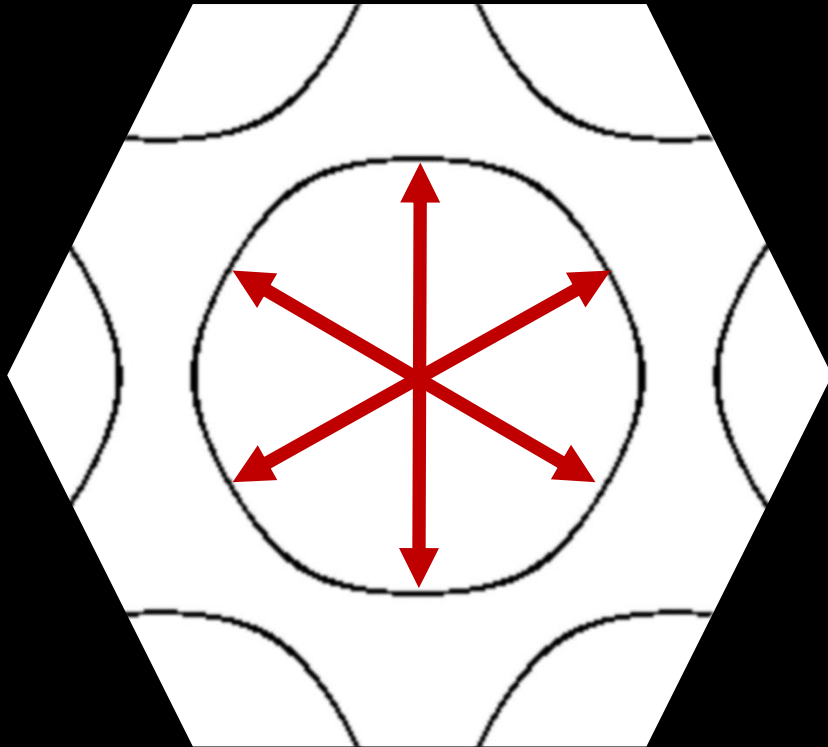
- Band structure from tight binding model (fit from ARPES data)
- No inter-plan interactions

$$H_{BdG} = \sum_{\langle i,j \rangle} t_{ij} (\hat{c}_{i\uparrow}^\dagger \hat{c}_{j\uparrow} + \hat{c}_{i\downarrow}^\dagger \hat{c}_{j\downarrow}) + \sum_i \Delta (\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger + \hat{c}_{i\downarrow} \hat{c}_{i\uparrow})$$

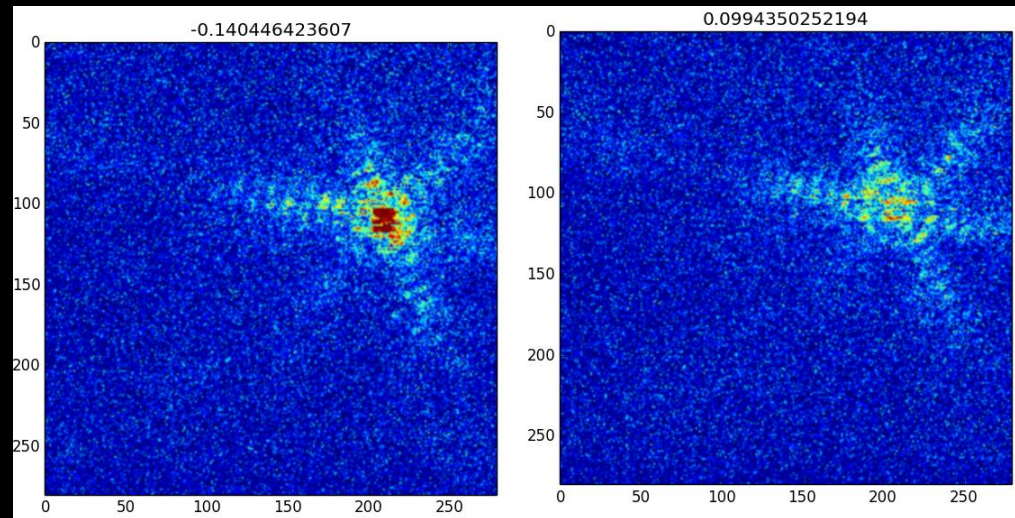
Comparison with joint-DOS calculations



Comparison with joint-DOS calculations

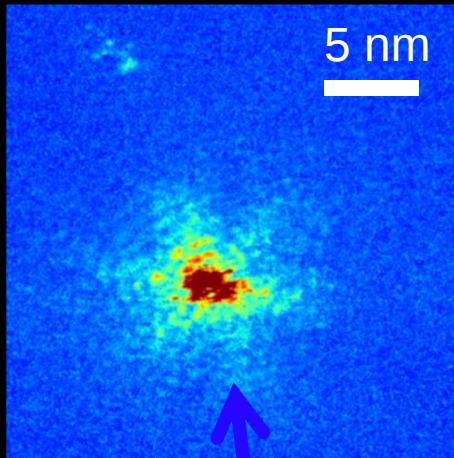


Joint DOS calculation indicate that the relevant part of the Fermi surface is the inner pocket.

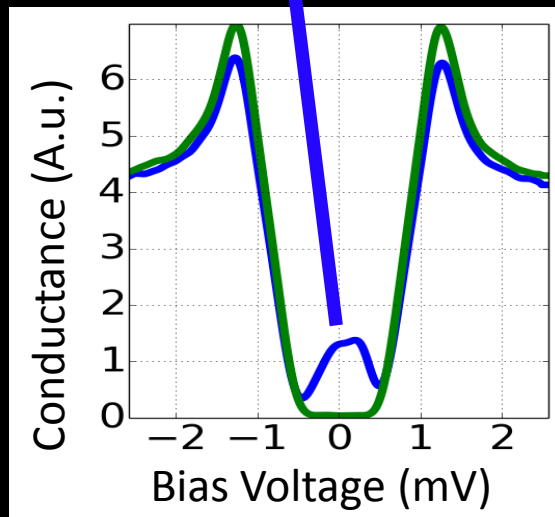


Two different impurities

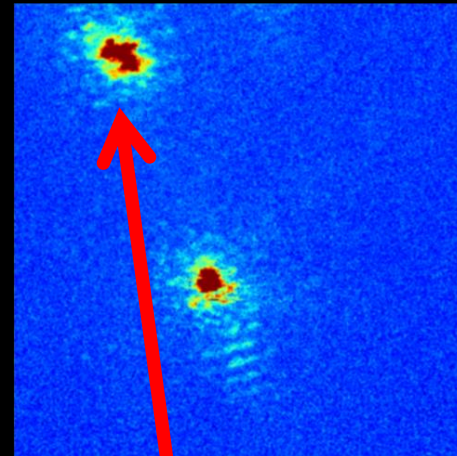
-0,12 meV



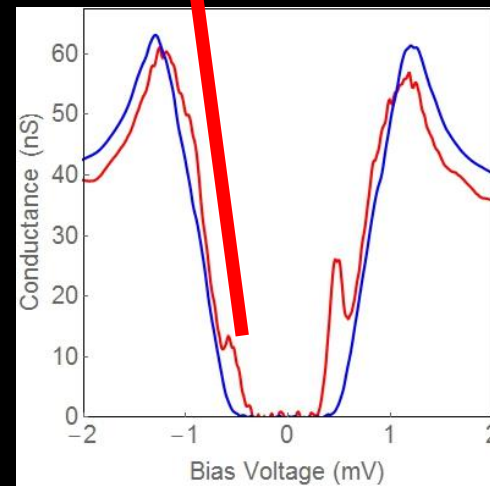
Cr?



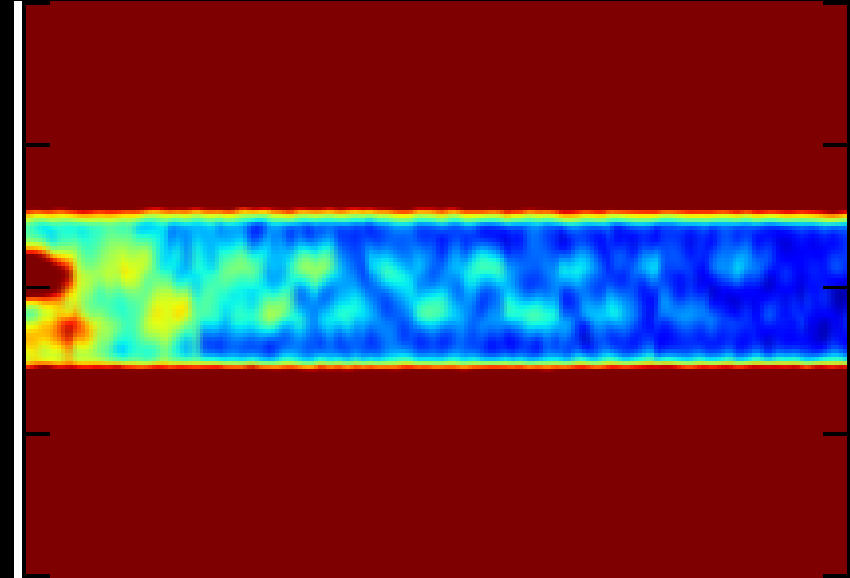
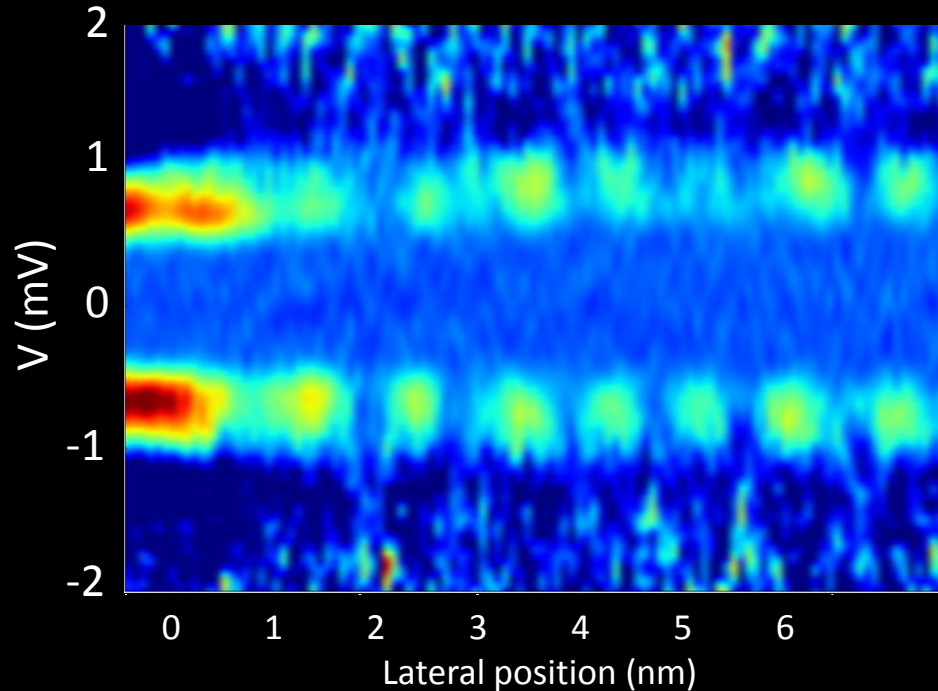
-0,34 meV



Mn?



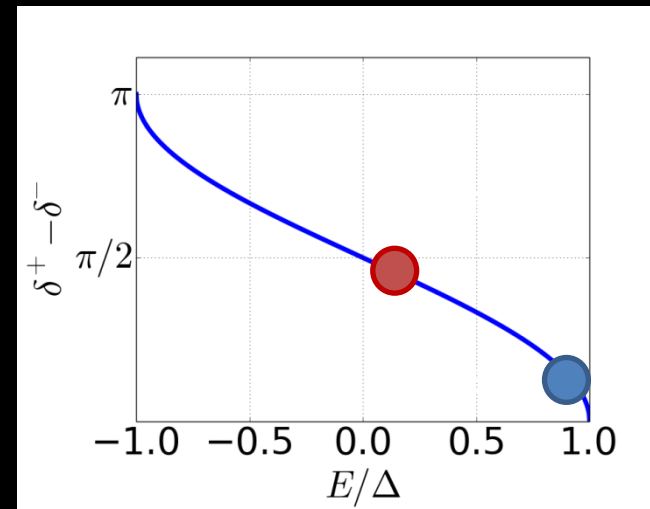
Impurity with bound states at gap edge: in phase electron-hole oscillations



$$\psi_{\pm}(r) = \frac{1}{\sqrt{N\pi k_F r}} \sin\left(k_F r - \frac{\pi}{4} + \delta^{\pm}\right) e^{-\Delta \sin(\delta^{+} - \delta^{-}) r / \hbar v_F}$$

$$E = \Delta \cos(\delta^{+} - \delta^{-})$$

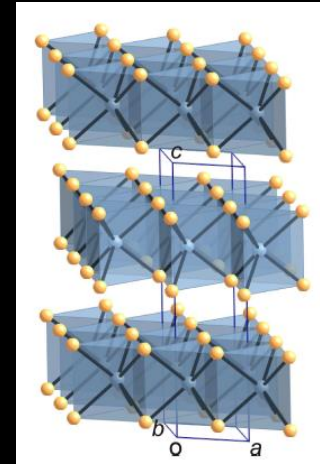
$$\tan \delta^{\pm} = (K\nu_0 \pm \nu_0 JS/2)$$



Two-dimensionnal superconductors

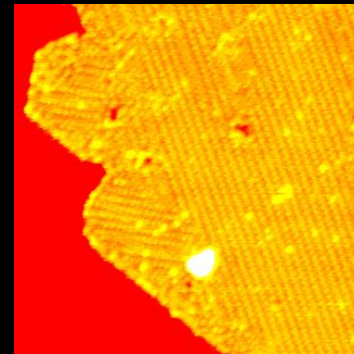
- Bulk superconductor with 2D electronic structure:

Lamellar material 2H-NbSe_2



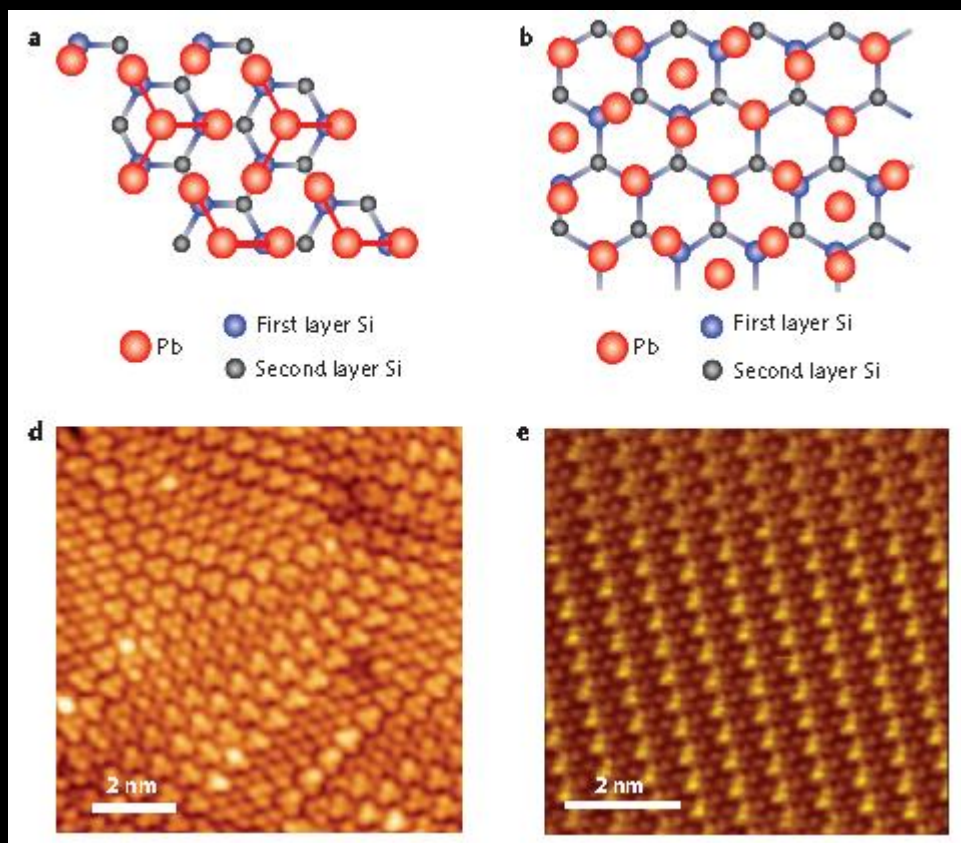
- Ultimately thin superconductor :

Single atomic layer of Pb/Si(111)



Superconductivity in a monolayer of Pb/Si(111)

*S. Zhang et al.
Nature Physics
6, 104 (2010)*

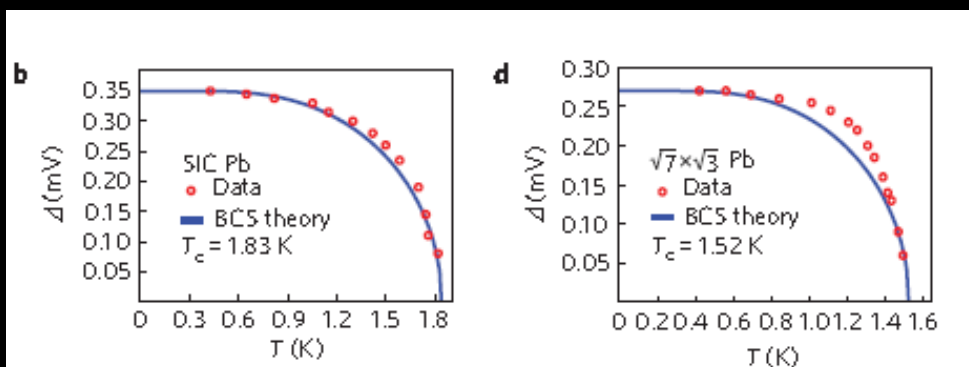


*Striped-
incommensurate
Pb/Si(111)*

1.33 monolayer

*$\sqrt{7} \times \sqrt{3}$
reconstruction of
Pb/Si(111)*

1.20 monolayer

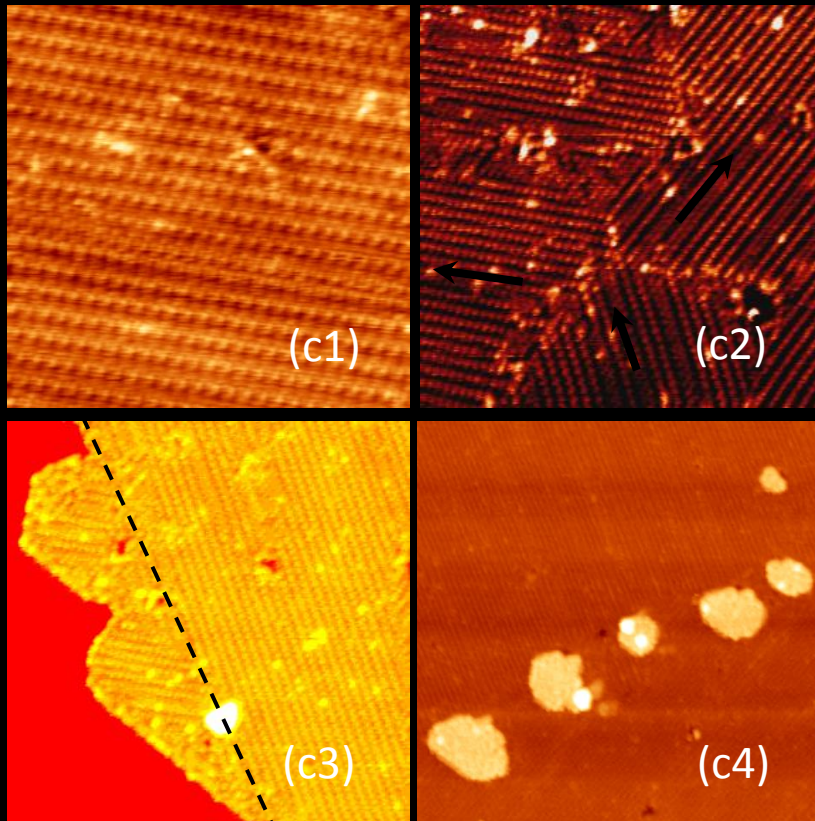


*In situ transport
 $R < \sim 1 \text{ k}\Omega$*

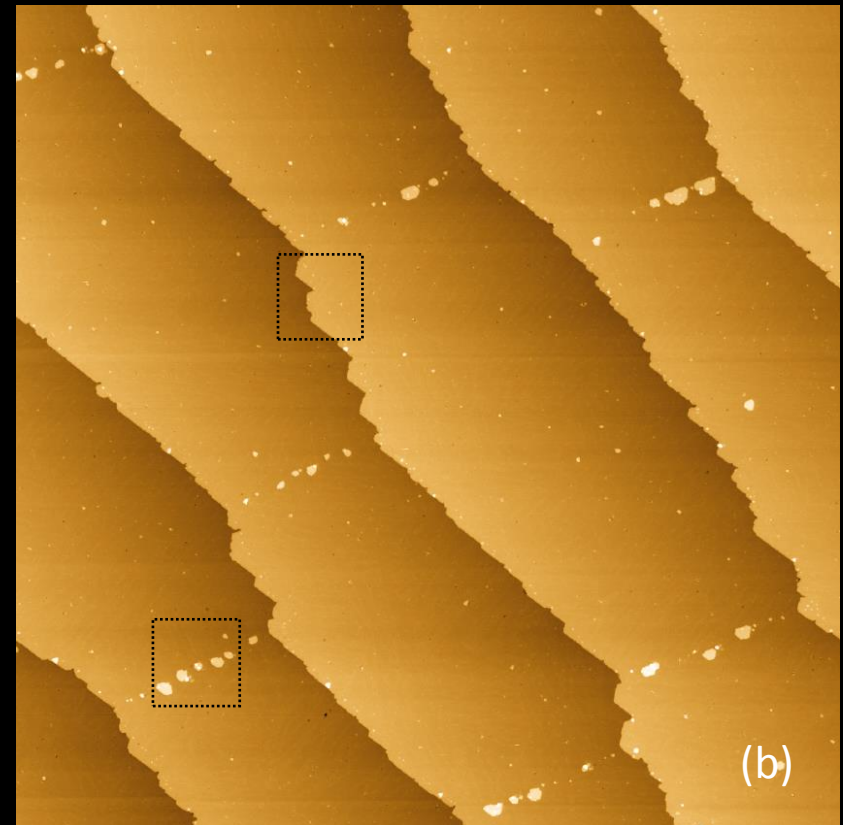
Electron Confinement in one Pb monolayer

1ML $\sqrt{7} \times \sqrt{3}$ Pb on Si(111)

Characteristic atomic defects



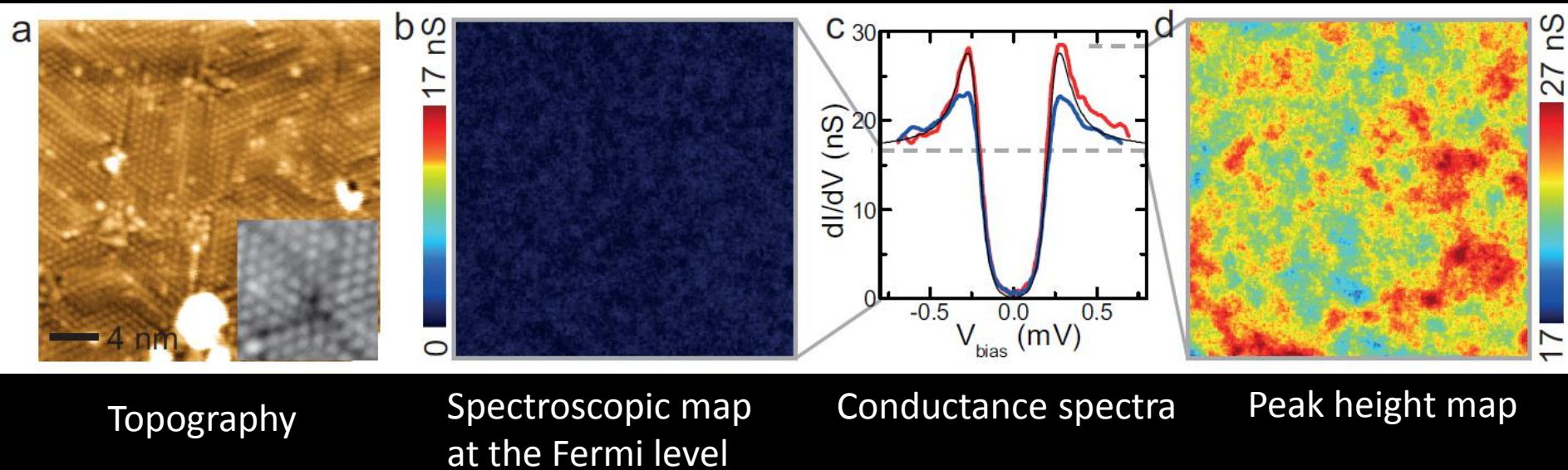
$\sqrt{7} \times \sqrt{3}$ Pb / Si(111)



600x600 nm²

Superconductivity vs Disorder in 1ML of Pb on Si(111)

Striped-Incommensurate Pb/Si(111) 1.33 monolayer



Fluctuation of the coherence peaks height on

$$\ell_{\text{fluct}} = 5 \text{ nm} < \xi_{\text{eff}} \sim 50 \text{ nm}$$

C. Brun et al. Nat. Phys. 10, 444 (2014)

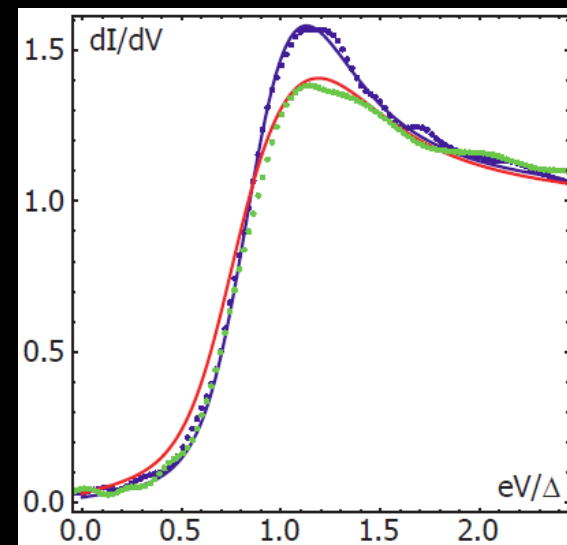
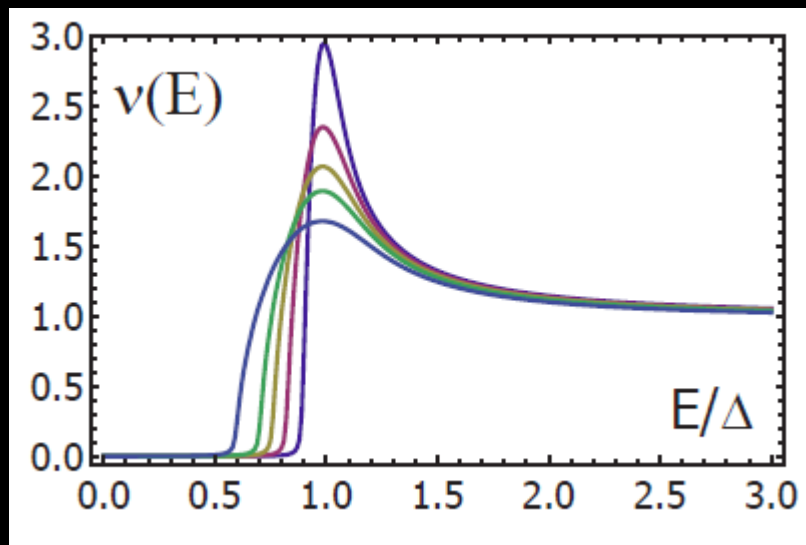
Fluctuation of the coherence peaks height

$$\ell_{\text{fluct}} = 5 \text{ nm} \ll \xi_{\text{eff}} \sim 50 \text{ nm}$$
$$\ell \sim 4 \text{ nm}, k_F \ell > 10-20$$

According to Lev Ioffe & Boris Altshuler:

Non BCS corrections due to the low dimensionnality and small mean free path (Real contact interaction instead of BCS reduced hamiltonian)

Indication of a possible BEC –BCS crossover

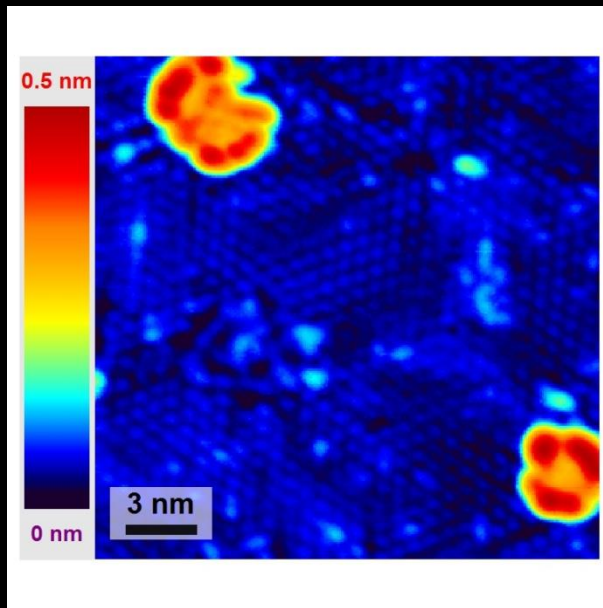


C. Brun et al. Nat. Phys. 10, 444 (2014)

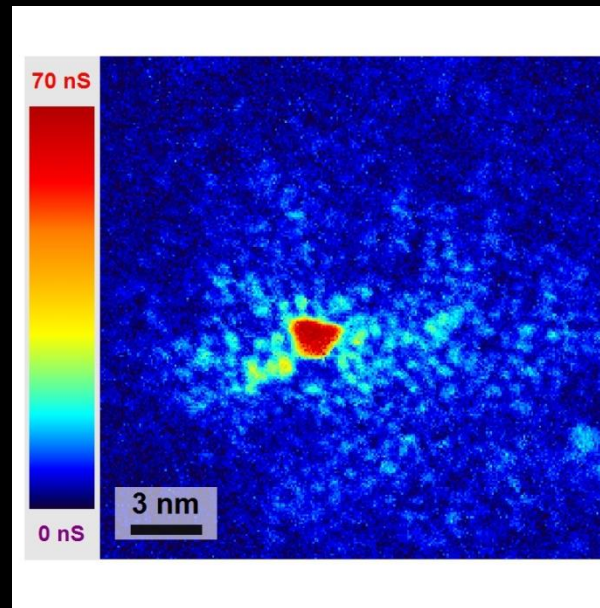
$G/G_Q \sim 30-100$

Shiba bound states in the stripe incommensurate monolayer of Pb/Si(111)

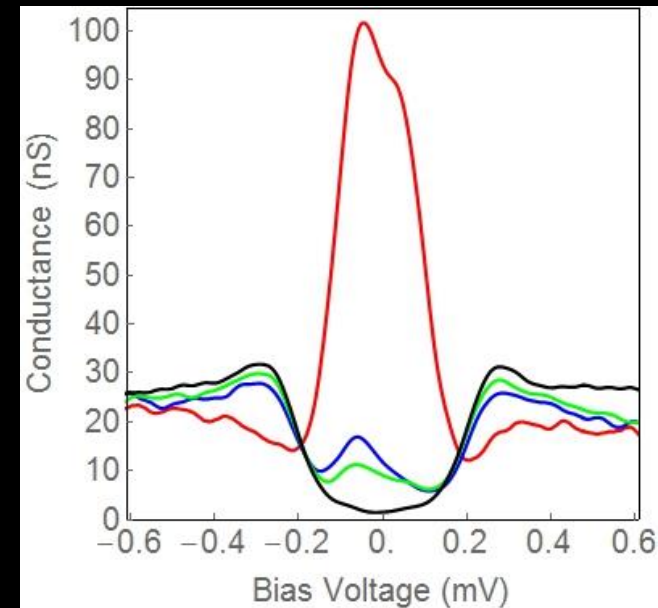
Striped-Incommensurate Pb/Si(111), 1.33 monolayer



Topography



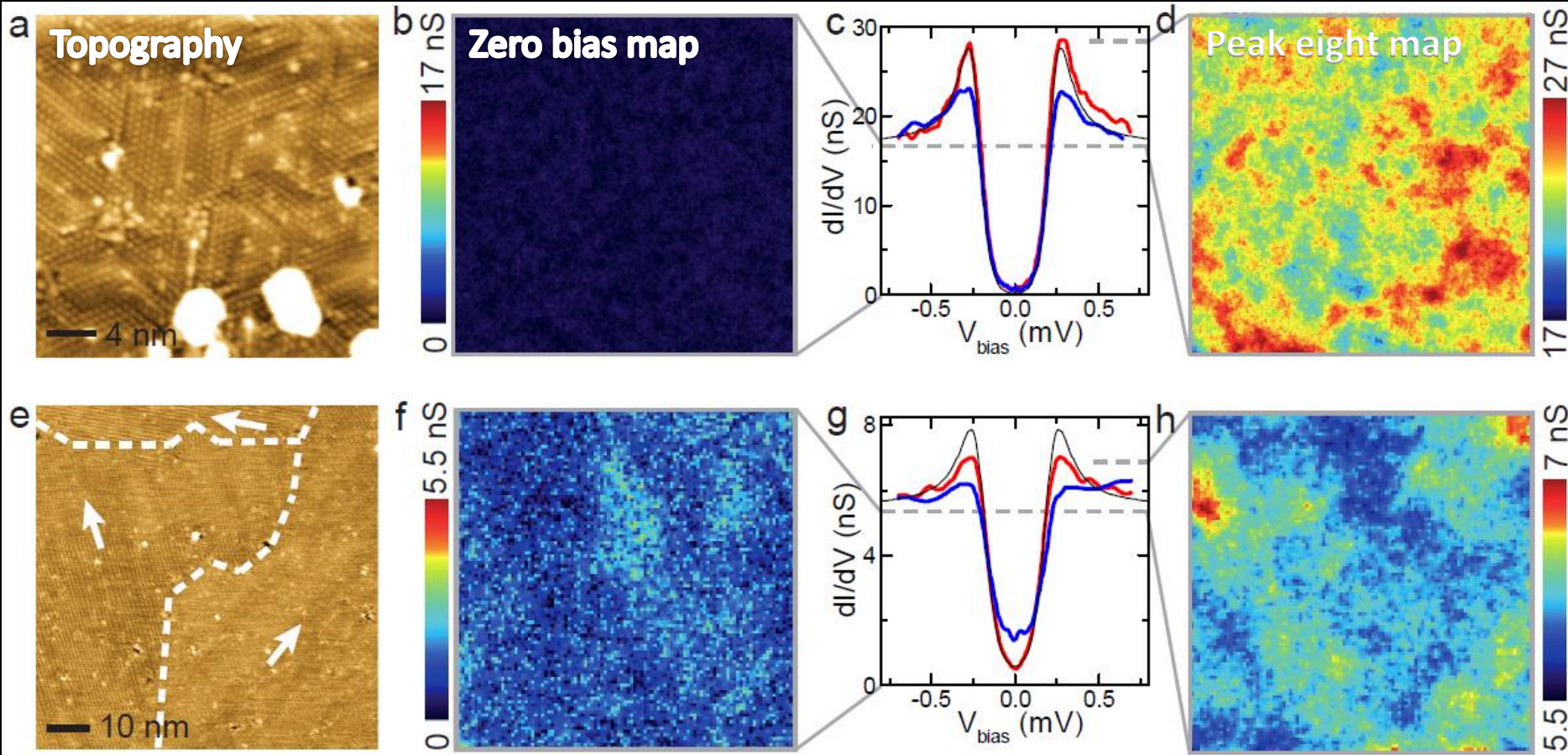
Conductance map at 0 mV



Conductance spectra on top (red), at 5 nm (blue), 10 nm (green) and far from the impurity (black)

Effect of non-magnetic disorder on the superconductivity of a single atomic layer of Pb/Si(111)

Striped-Incommensurate Pb/Si(111), 1.33 monolayer



$\sqrt{3} \times \sqrt{7}$ -Pb/Si(111), 1.2 monolayer

C. Brun et al. Nat. Phys. 10, 444 (2014)

Gap filling and fluctuations of zero bias conductance in $\text{Pb}/\sqrt{7} \times \sqrt{3}$

- Strong spin-orbit coupling in $\text{Pb}/\text{Si}(111)$ monolayer due to the non-centrosymmetry at the surface
- Superconductivity develops on a Rashba splitted ground state

Superconducting 2D System with Lifted Spin Degeneracy: Mixed Singlet-Triplet State

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Origin of the gap filling in $\sqrt{7}\times\sqrt{3}$ -Pb/Si(111)

Superconducting 2D System with Lifted Spin Degeneracy: Mixed Singlet-Triplet State

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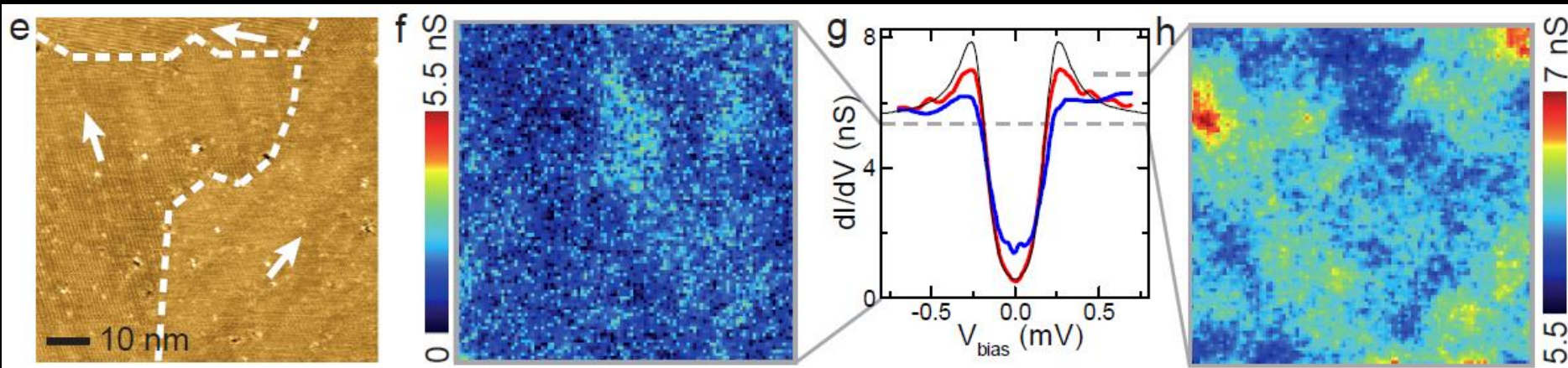
National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310

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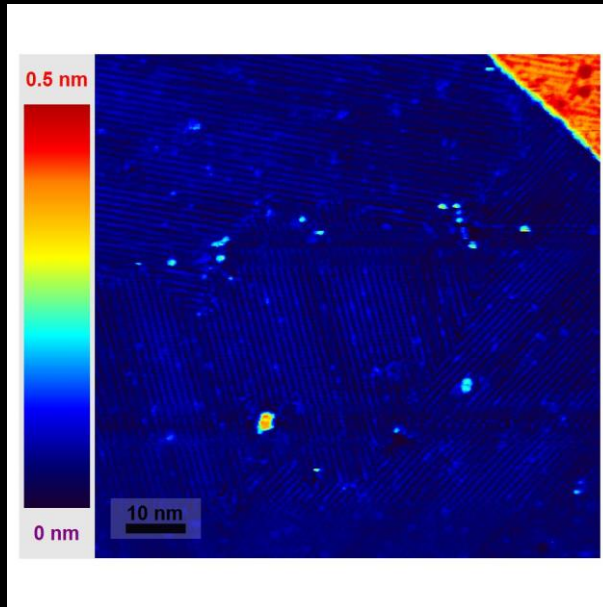
Department of Physics, The State University of New York at Buffalo, Buffalo, New York 14260

Gor'kov and Rashba PRL 87, 037004 (2001)

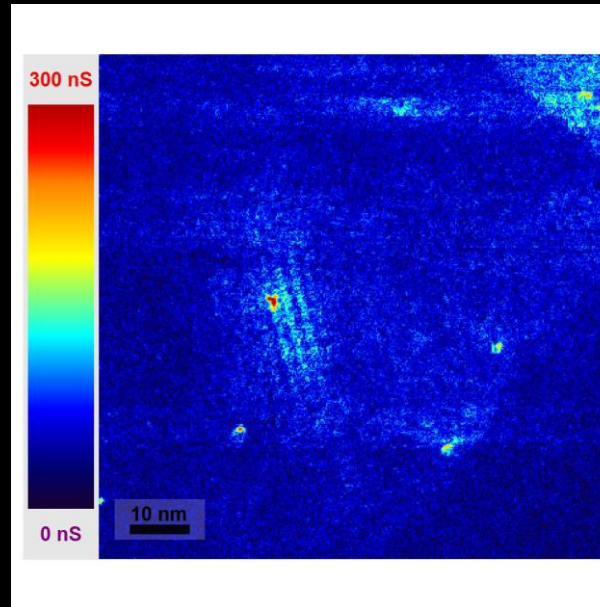
The triplet part is sensitive to non-magnetic disorder
(Analogous to weak magnetic disorder in a s-wave superconductor)



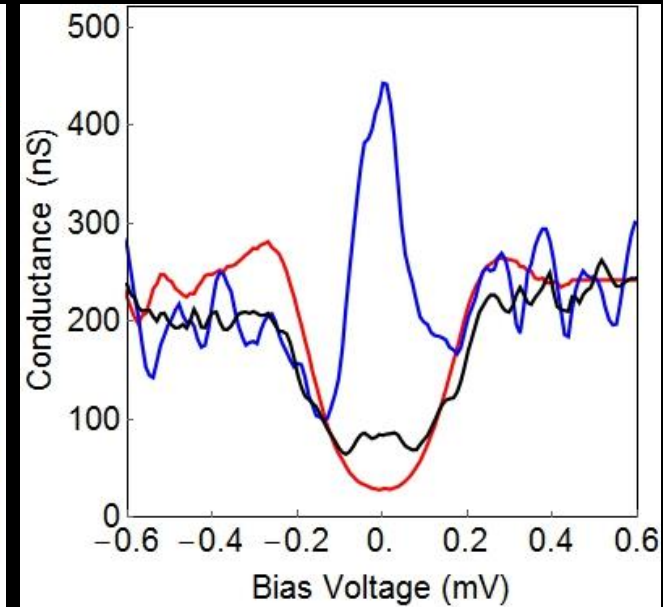
Extended bound states around magnetic defects in $\sqrt{3} \times \sqrt{7}$ -Pb/Si(111)



Topography



Conductance map at 0 mV



Conductance spectra on top (red), at 5 nm (blue), 10 nm (green) and far from the impurity (black)

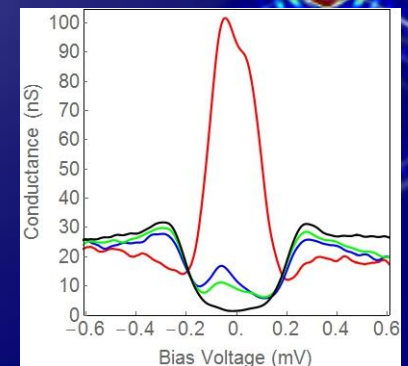
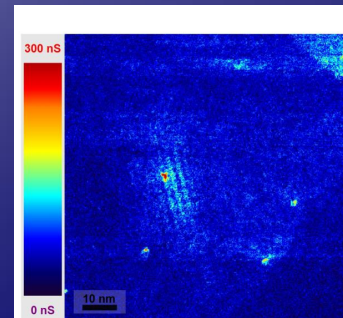
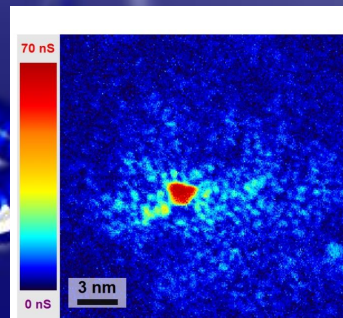
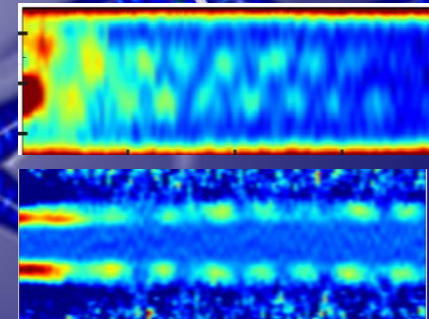
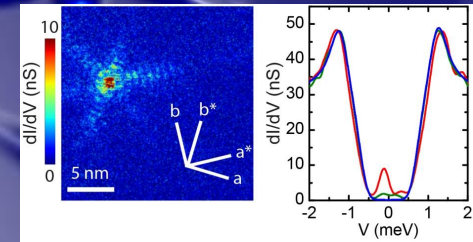
Coupling a classical spin to a 2D condensate leads to spatially extended, quantum coherent, spin polarized, bound states

- Large star shaped bound states in NbSe₂

- Oscillating electron-hole asymmetry

- Phase shift governed by bound state energy

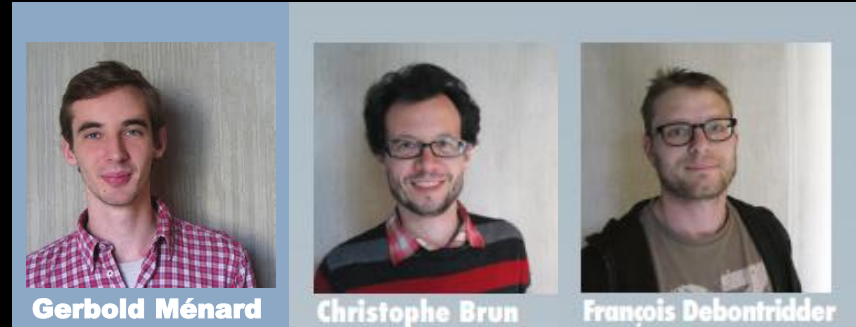
- Very large extend of Yu-Shiba-Rusinov bound states in Pb/Si(111) monolayers



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- Étienne Janod



Thank you !