Odd-frequency pairing induced by magnetic impurities in a superconductor

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Pairing function

Key quantity: the pairing correlation is defined by:

$$F_{\alpha,\beta}(\boldsymbol{r}_1 t_1, \boldsymbol{r}_2 t_2) = -i \left\langle \mathsf{T} \psi_\alpha(\boldsymbol{r}_1 t_1) \psi_\beta(\boldsymbol{r}_2 t_2) \right\rangle$$

Under exchange of the two electrons, it must satisfy:

$$F_{\alpha,\beta}(\boldsymbol{r}_1 t_1, \boldsymbol{r}_2 t_2) = -F_{\beta,\alpha}(\boldsymbol{r}_2 t_2, \boldsymbol{r}_1 t_1)$$

Even/odd-frequency pairing

Key quantity: the pairing correlation is defined by:

$$F_{\alpha,\beta}(\boldsymbol{r}_1 t_1, \boldsymbol{r}_2 t_2) = -i \left\langle \mathsf{T} \psi_\alpha(\boldsymbol{r}_1 t_1) \psi_\beta(\boldsymbol{r}_2 t_2) \right\rangle$$

Under exchange of time:

Conventional even-frequency pairing:

$$F_{\alpha,\beta}(\boldsymbol{r}_1 t_1, \boldsymbol{r}_2 t_2) = F_{\alpha,\beta}(\boldsymbol{r}_1 t_2, \boldsymbol{r}_2 t_1)$$

odd-frequency pairing :

$$\boxed{F_{\alpha,\beta}(\boldsymbol{r}_1 t_1, \boldsymbol{r}_2 t_2) = -F_{\alpha,\beta}(\boldsymbol{r}_1 t_2, \boldsymbol{r}_2 t_1)}$$

V. L. Berezinskii, *JETP Lett.* 20, 287 (1974)

Symmetry of the pairing function

Orbital ⊗ Spin ⊗ Frequency = Odd

Several options

	Frequency (time)	Spin	Orbital	Total
ESE	+(even)	− (singlet)	+(even)	−
ETO	+(even)	+ (triplet)	−(odd)	−
OTE	−(odd)	+ (triplet)	+(even)	−
OSO	−(odd)	− (singlet)	−(odd)	−

BCS; cuprates (ESE)

P-wave SC => Majoranas (ETO)

See e.g. Y. Tanaka, M. Sato, N. Nagaosa, J. Phys. Soc. Jpn. 81, 011013 (2012)
J. Linder, A. V. Balatsky, Rev. Mod. Phys. 91, 045005 (2019)

A long history….

Odd-frequency pairing was proposed

- First by Berezinskii in 74' (superfluid He)

- As a purely intrinsic electronic mechanism to generate bulk odd-ω spin triplet pairing

  Belitz, Kirkpatrick, 91',92'
  Balatsky, Abrahams, 91',92', etc.

- In the Kondo lattice and heavy fermions

  Zachar, Emery, Kivelson, 96',
  Coleman, Miranda, Tsvelik, 97'; etc.

- In hybrid SF junctions, odd-ω pair amplitudes are induced in a ferromagnet in contact with a spin-singlet s-wave superconductor

  Bergeret, Efetov, Volkov, 01'

See e.g. **Y. Tanaka, M. Sato, N. Nagaosa, J. Phys. Soc. Jpn. 81, 011013 (2012)**

J. Linder, A. V. Balatsky, Rev. Mod. Phys. 91, 045005 (2019)

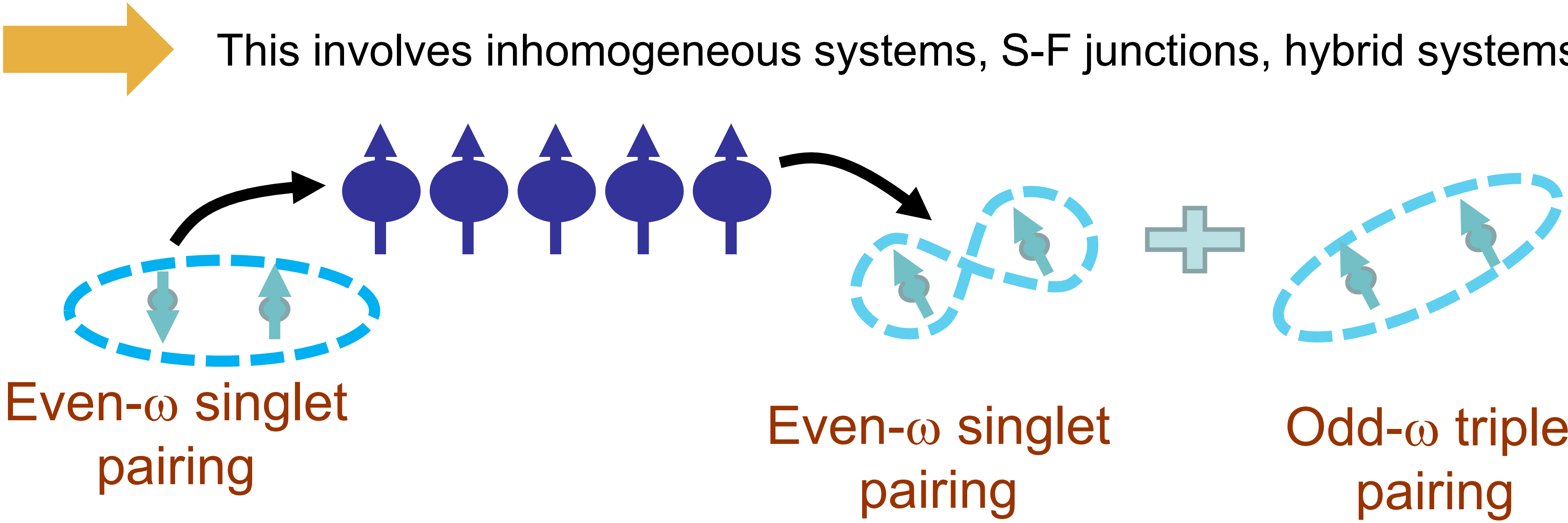
1D case: **J. Cayao, C. Triola, A. M Black-Schaffer, The European Physical Journal Special Topics, 229, 545 (2020)**

Where to find it ?

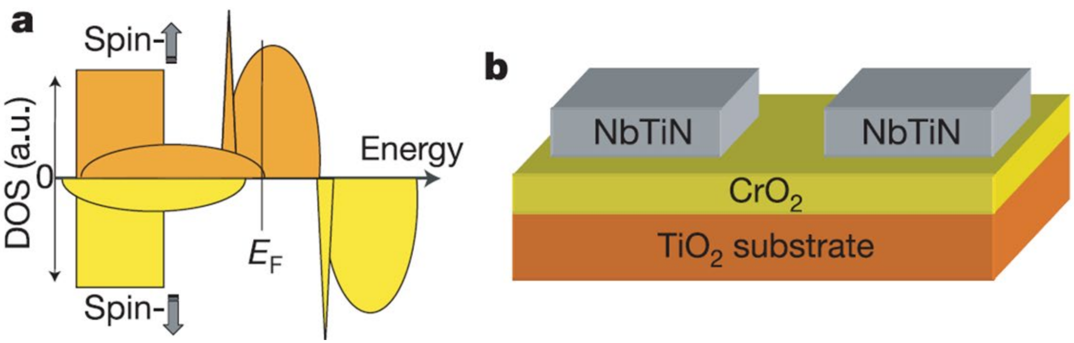
Actually, odd-ω pairing state is rather ubiquitous:

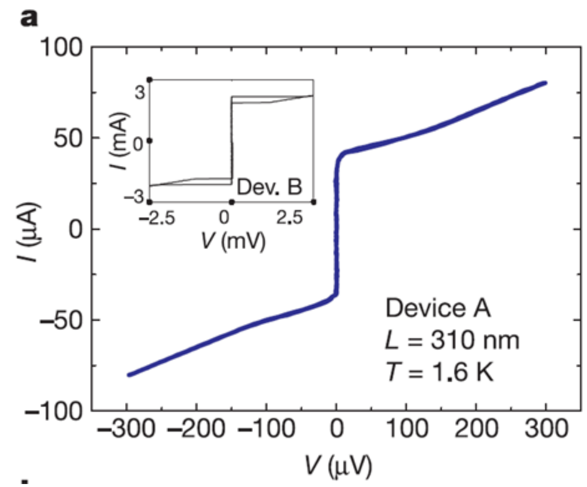
Starting from conventional s-wave even-ω superconductivity, any system with broken spin rotational symmetry OR broken translation symmetry can induce odd-ω pairing state.

This involves inhomogeneous systems, S-F junctions, hybrid systems….



Odd-w pairing in ferromagnet-superconductor hybrid systems





Long range proximity effect in a S-F-S junction as a direct manifestation of odd triplet s-wave pairing

R. S. Keizer et al., Nature 439, 825 (2006)

Outline

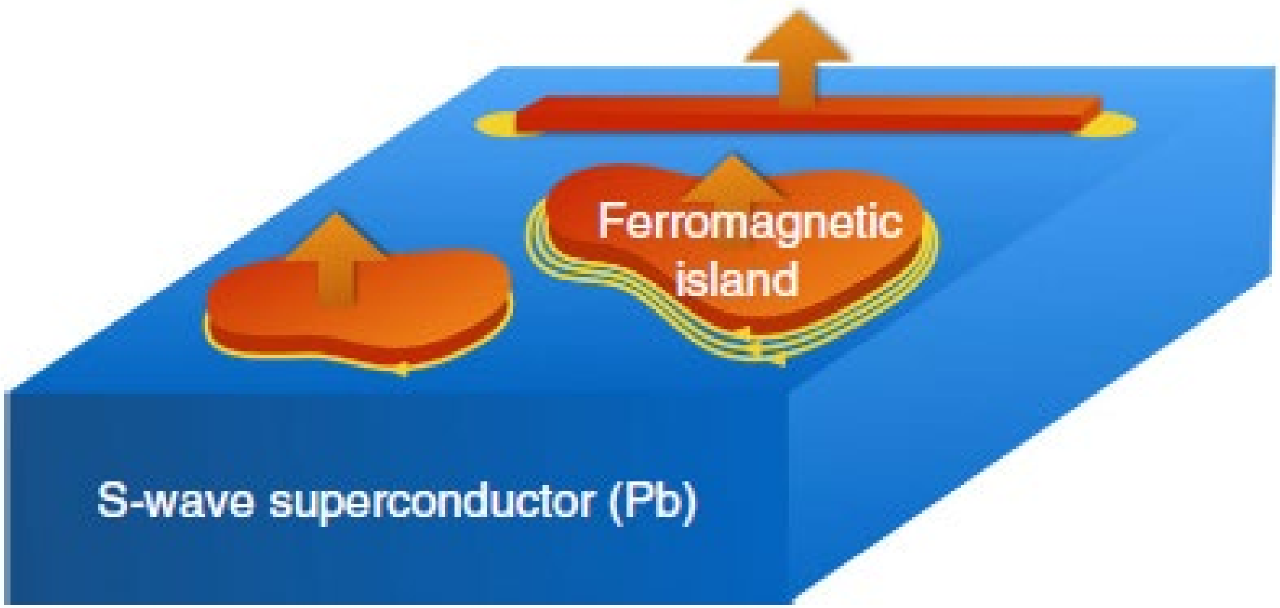
I) Interplay between magnetism and superconductivity:
a rich playground for topological superconductivity

II) Odd-frequency pairing generated by a single magnetic impurity

I) Interplay between magnetism and superconductivity:

a rich playground for topological superconductivity

Topological superconductivity in ferromagnet-superconductor hybrid systems

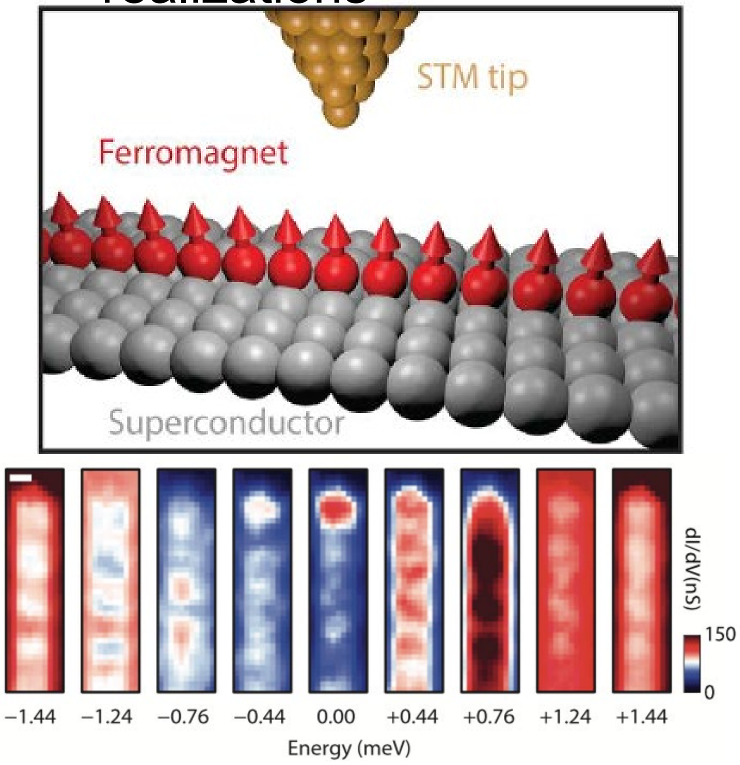


Jian Li et al., Nature Communications 7, 12297 (2016)

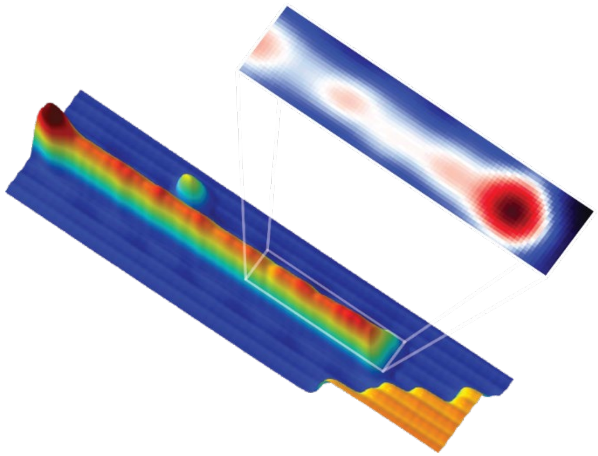
Majorana end states around 1D magnetic chains

Chain/wire of magnetic adatoms

Possible experimental realizations



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

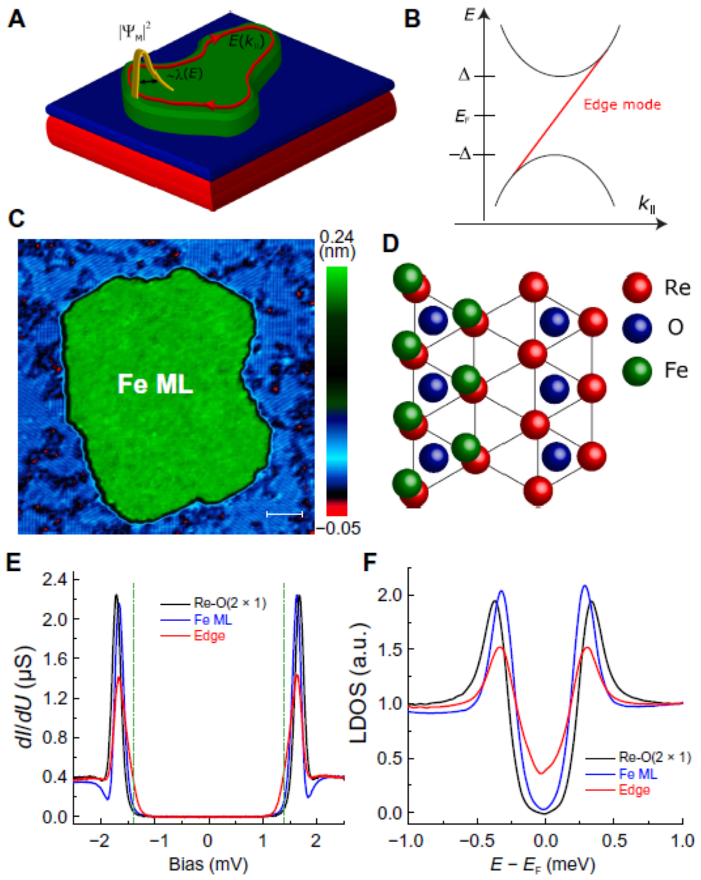


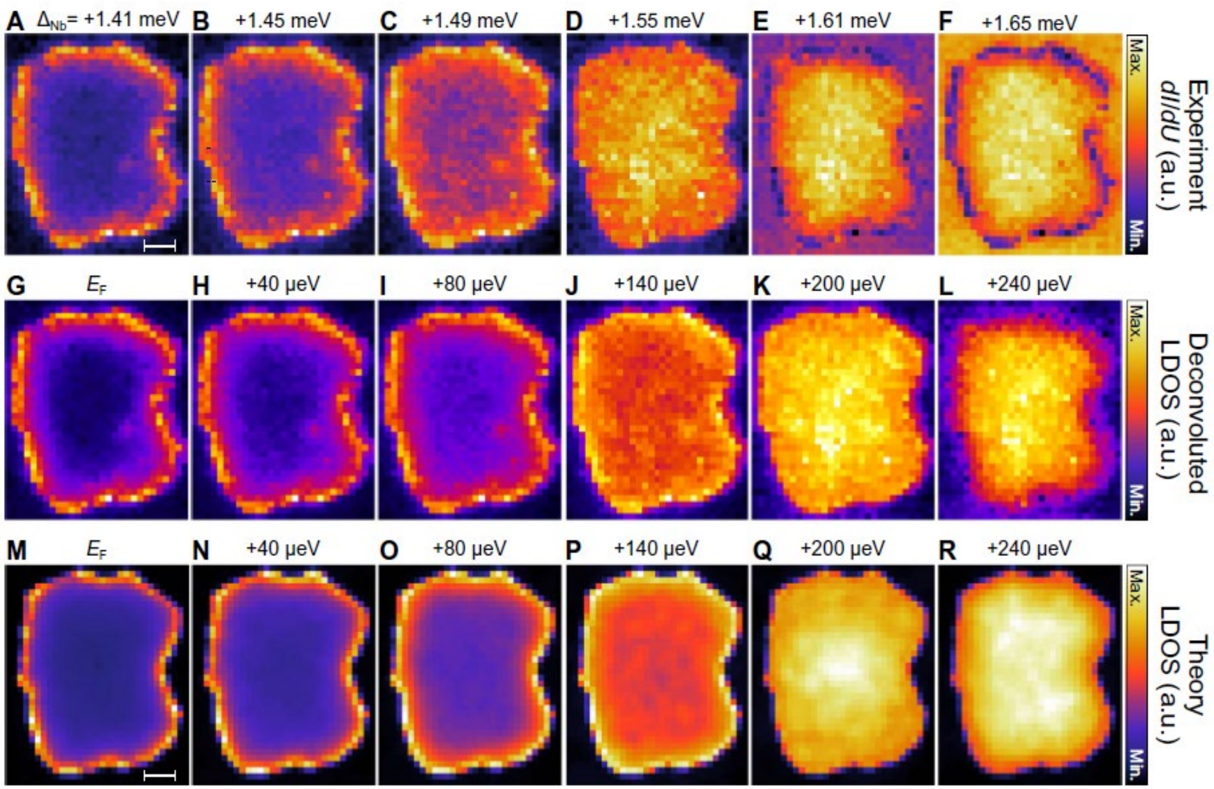
S. Nadj-Perge et al., Science **346,** 6209 (2014)
B. E. Feldman et al., Nature Physics (2016)
S. Jeon et al., Science (2017) **(Princeton)**

see also

M. Ruby et al., PRL 2015 **(Berlin)**
R. Pawlak et al., NPJ QI (2016) **(Basel)**
H. Kim et al. Science Advances (2018) **(Hamburg)**

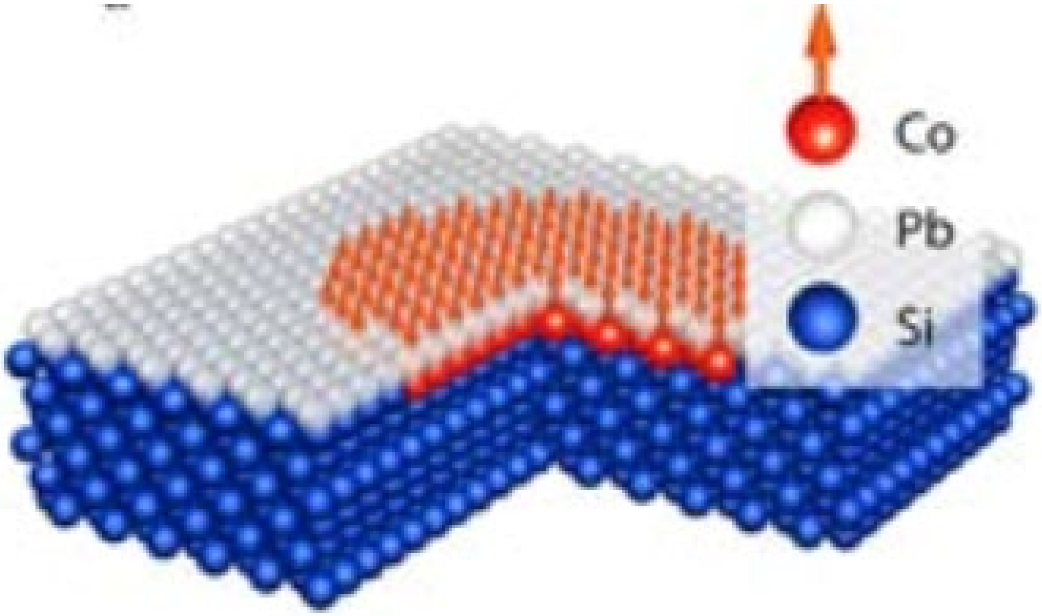
Dispersive edge modes in Fe/Re





Palacio-Morales et al. Science Advances (2019) **(Hamburg)**

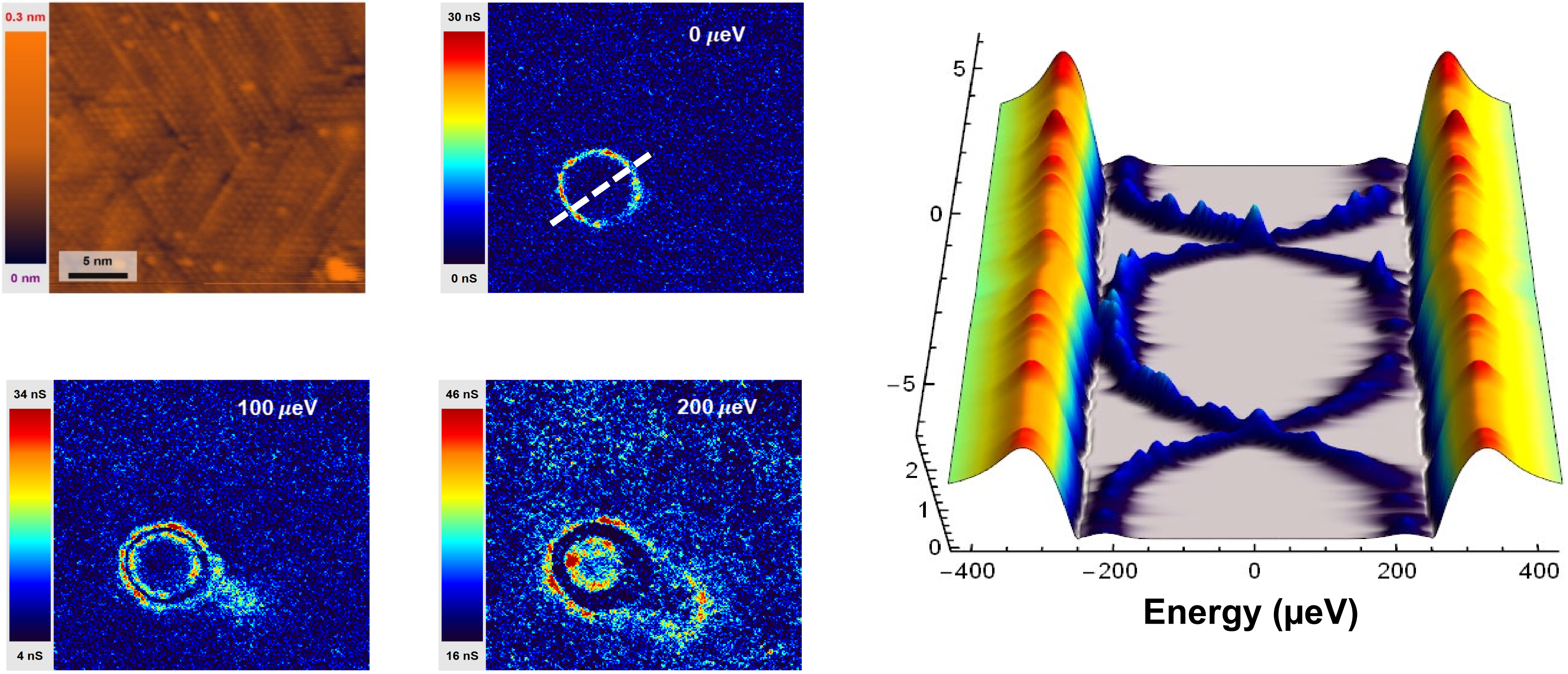
2D topological superconductivity in a Pb monolayer



Pb/Si(111) Rashba superconductor coupled to a ferromagnetic domain

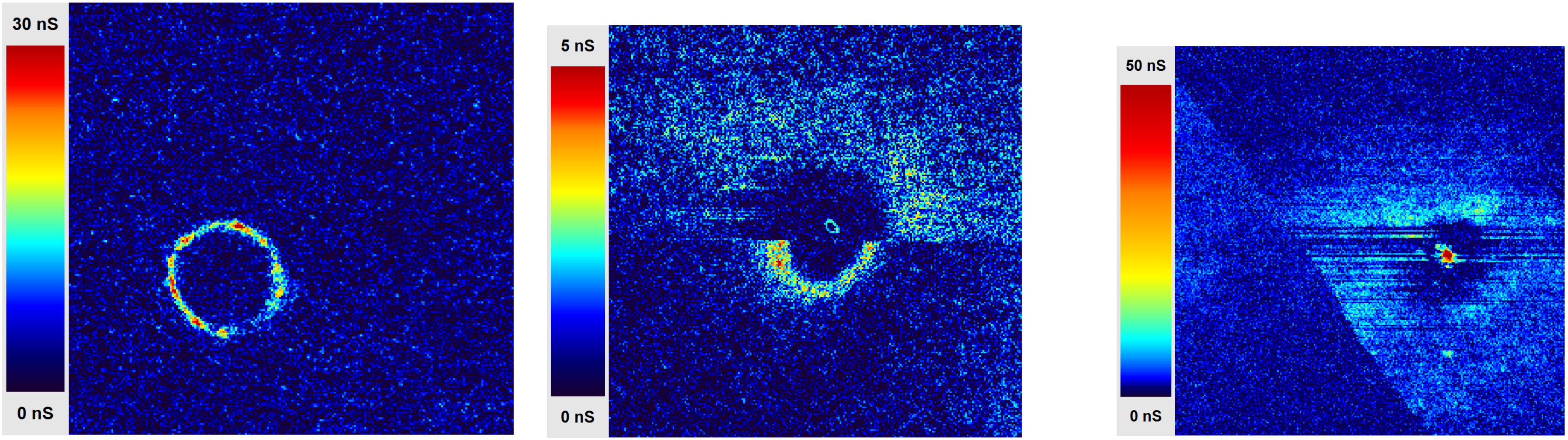
G. Ménard et al., Nature Comm. 8, 2040 (2017)

Dispersive edge states in Pb/Co/Si(111)



G. Ménard et al., Nature Comm. 8, 2040 (2017)

Switching to zero energy bound states



Conductance maps at zero energy (H = 0 mT, T = 320 mK)

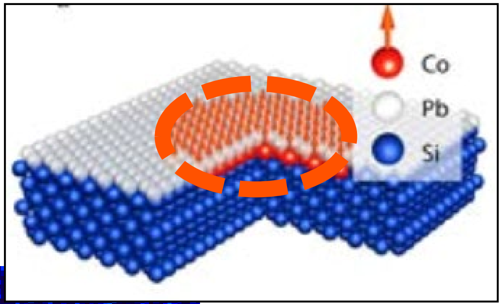
The system spontaneously switches to a new configuration with two zero energy bound states:

- A zero bias bound state in the center
- A zero bias partner on the the rim

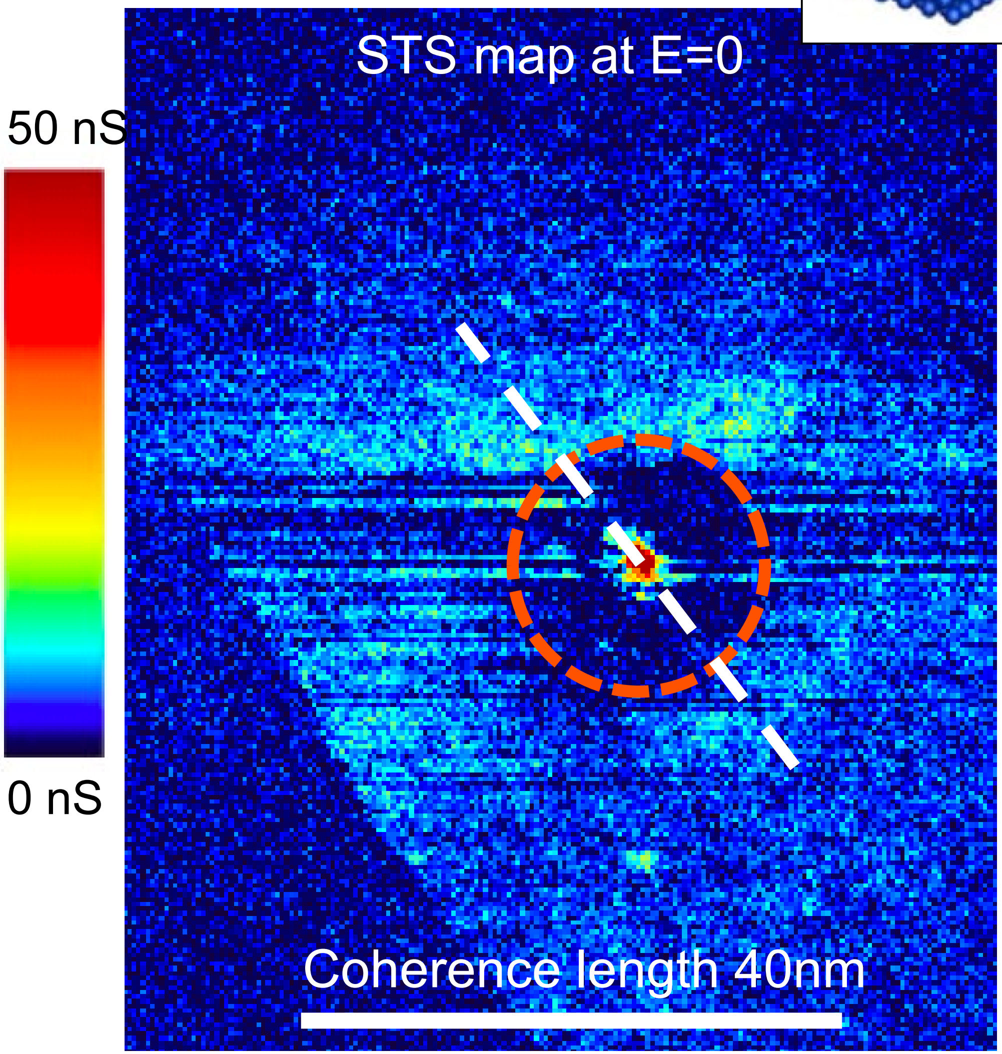
Ménard et al., Nature Comm. 10, 2587 (2019)

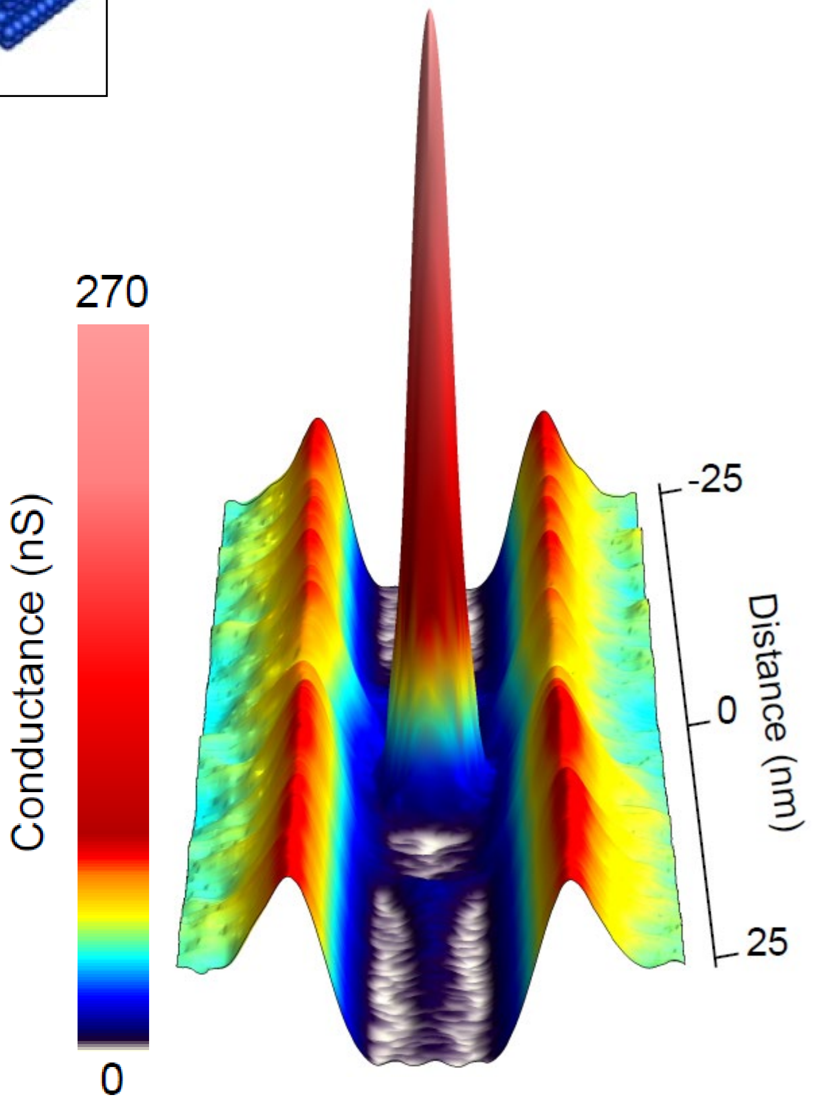
Pair of zero energy states

(1) Strongly localized + edge state



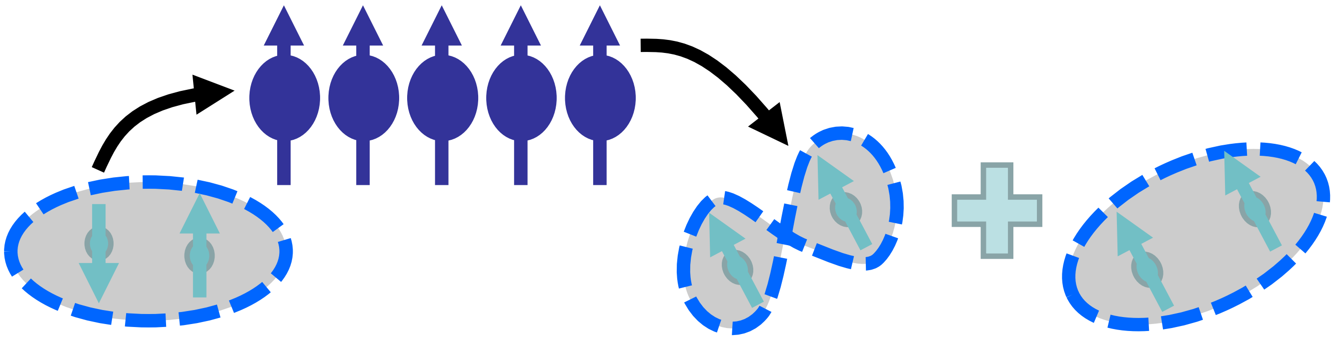
(2) Isolated in energy





Ménard et al, Nature Comm (2019)

Topological vs odd-ω triplet superconductivity in hybrid systems

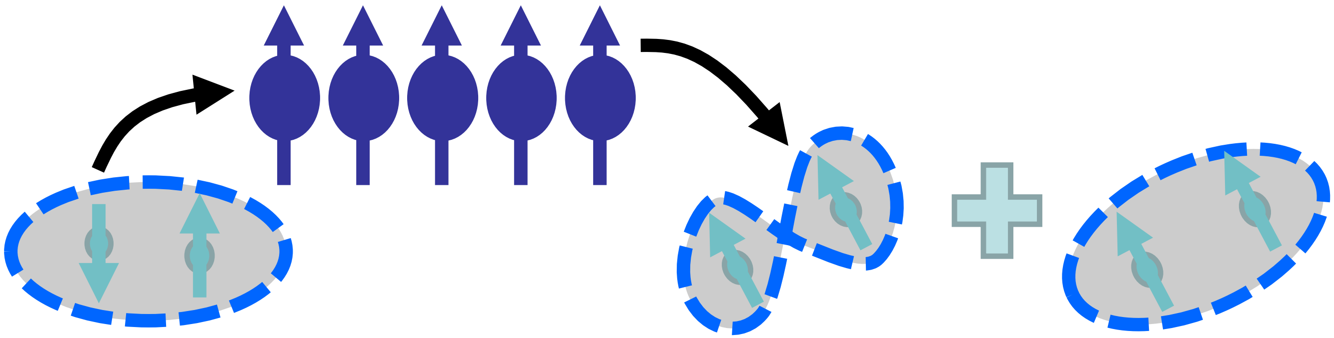


Complex problem !!!

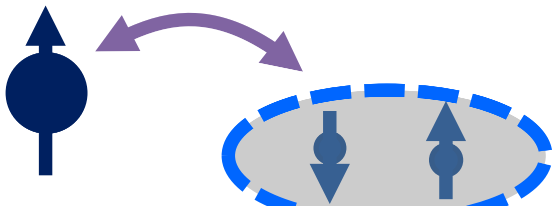
Symmetry and Topology in Superconductors - Odd-frequency pairing and edge states
Y. Tanaka, M. Sato, N. Nagaosa, J. Phys. Soc. Jpn. 81, 011013 (2012)

Our strategy: back to basis, try to understand a simpler problem

Topological vs odd-ω triplet superconductivity in hybrid systems

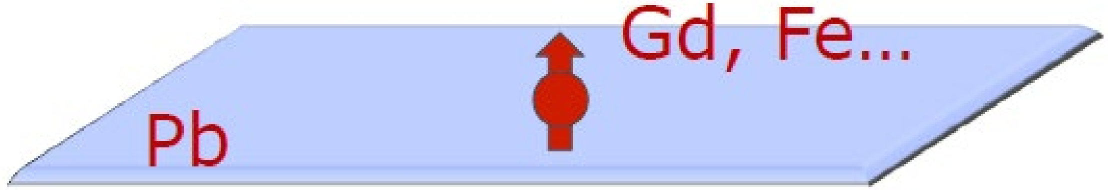


Odd-triplet correlations induced by a single magnetic atom



II) Odd-ω frequency pairing generated by a single magnetic impurity

A magnetic impurity in a superconductor



Bogoliubov-de Gennes Ham. $\mathcal{H}_0 = \xi_p \tau_z + \Delta \tau_x$

Spin impurity Ham. $\mathcal{H}_{\mathrm{imp}} = -J\mathbf{S} \cdot \sigma \; \delta(\mathbf{r})$

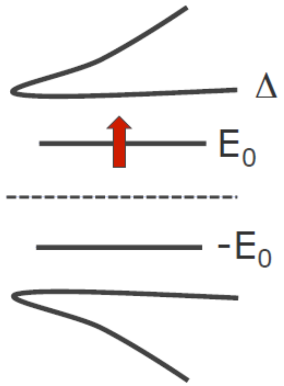
Consider the classical spin limit S>>1

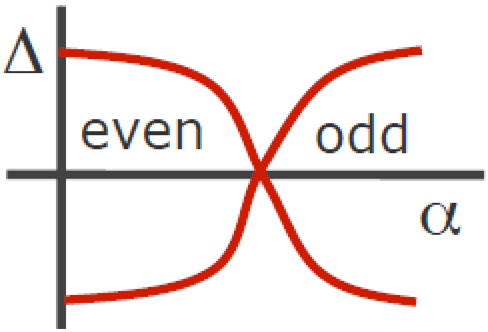
$\Rightarrow$ $\mathcal{H}_{\mathrm{imp}} = -JS\sigma^z \; \delta(\vec{r})$ **Like a local magnetic field**

Shiba in-gap bound state:

$$E_0 = \Delta \frac{1-\alpha^2}{1+\alpha^2}$$

$$\alpha = \pi \nu_0 J S$$





Yu Lu (1965), Shiba (1968), Rusinov (1968)

Shiba bound states in 2D superconductors

Convenient paramatrization

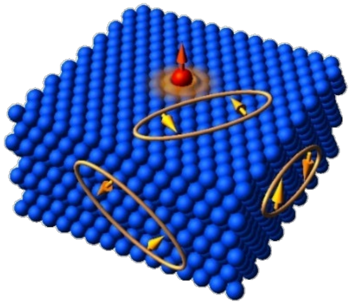
$$E = \Delta \cos(\delta^+ - \delta^-)$$

$$\tan \delta^\pm = (V\nu_0 \pm \nu_0 JS/2)$$

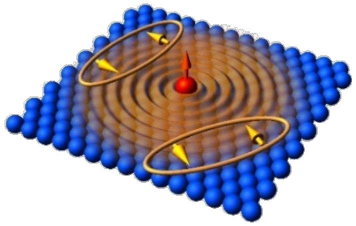
Rusinov (1969)

Potential scattering term

$$\psi_\pm^{3D}(r) = \frac{1}{\sqrt{N}} \frac{\sin\left(k_F r + \delta^\pm\right)}{r} e^{-\sin(\delta^+ - \delta^-) r/\xi}$$



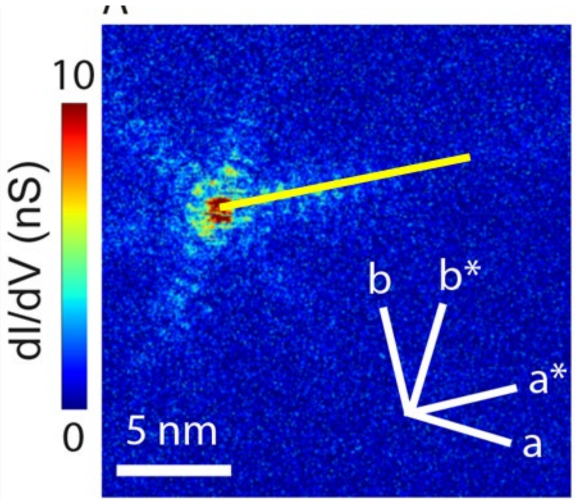
$$\psi_\pm^{2D}(r) = \frac{1}{\sqrt{N}} \frac{\sin\left(k_F r + \delta^\pm - \frac{\pi}{4}\right)}{\sqrt{r}} e^{-\sin(\delta^+ - \delta^-) r/\xi}$$

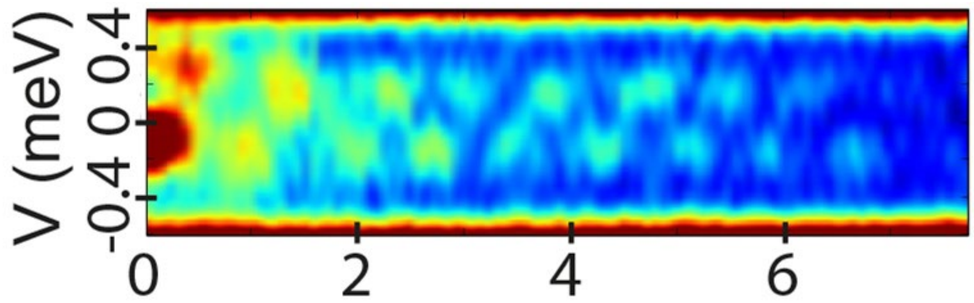


Lower dimensionality leads to **larger extents** of YSR bound states

G. Ménard et al., Nature Physics 11, 1013 (2015)

Shiba bound states around magnetic impurities in 2H-$NbSe_2$



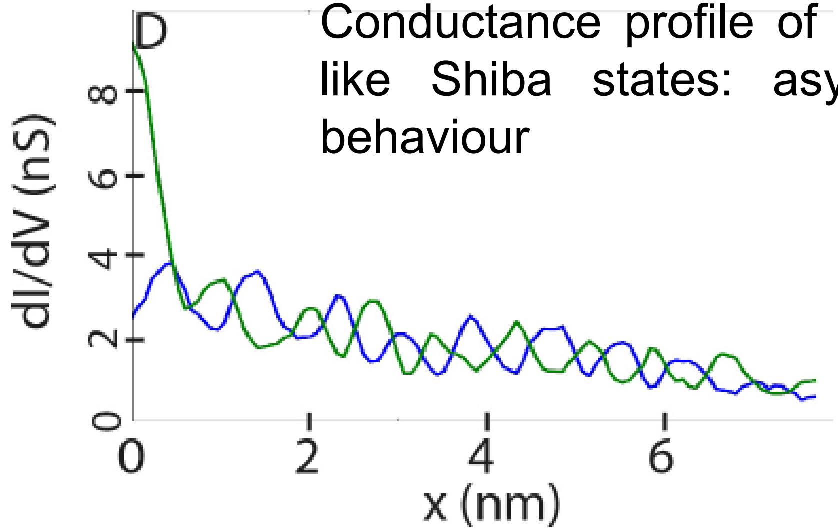


The Shiba peaks **position relatively to the gap** is directly related to the phase shift.

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

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

$$\tan \delta^\pm = (V\nu_0 \pm \nu_0 JS/2)\, 2)$$



Conductance profile of electron and holes like Shiba states: asymptotic antiphase behaviour

G. Ménard et al., Nature Physics 11, 1013 (2015)

Odd-Frequency Pairing on the impurity site

$$\hat{G}^R(t,t') = -i\theta(t-t')\langle\Psi(\mathbf{0},t)\Psi^\dagger(\mathbf{0},t')\rangle$$
$$= \begin{bmatrix} G^R_\uparrow(t-t') & F^R_{\uparrow,\downarrow}(t-t') \\ -F^R_{\downarrow,\uparrow}(t-t')^* & -G^R_\downarrow(t-t')^* \end{bmatrix}$$

Retarded Green function in Nambu space

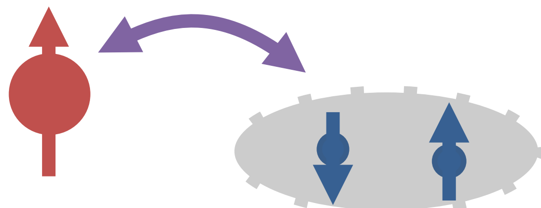
Dyson equation : $[\hat{G}^R]^{-1}(\omega) = [g^R(\omega)]^{-1} - \Sigma$

$$g^R(\omega) = \begin{bmatrix} g^R_\uparrow(\omega) & f^R_{\uparrow,\downarrow}(\omega) \\ f^R_{\uparrow,\downarrow}(\omega) & -(g^R_\downarrow(-\omega))^* \end{bmatrix} \qquad \hat{\Sigma} = \begin{bmatrix} V-J-i\Gamma & 0 \\ 0 & -(V+J)-i\Gamma \end{bmatrix}$$

Width of the bound state

Two possibilities:

1. $F^R_{\uparrow,\downarrow}(\omega) = F^{R*}_{\uparrow,\downarrow}(-\omega)$ Even ω; spin singlet,
2. $F^R_{\uparrow,\downarrow}(\omega) = -F^{R*}_{\uparrow,\downarrow}(-\omega)$ Odd ω; spin triplet.



Odd-Frequency Pairing on the impurity site

Local density of states on the impurity:

$$\rho_{\mathrm{even/odd}}(\omega) = [\rho(\omega) \pm \rho(-\omega)]/2$$

$$|\omega| < \Delta$$

$$\rho_{\mathrm{even/odd}}(\omega) = C_{e/o}(E_0) \times \Im F^R_{\mathrm{odd/even}}(\omega)$$

General proportionality relation between LDOS and the odd-ω pairing fuction

Odd-Frequency Pairing on the impurity site

Local density of states on the impurity:

$$\rho_{\text{even/odd}}(\omega) = [\rho(\omega) \pm \rho(-\omega)]/2$$

$$|\omega| < \Delta$$

$$\rho_{\text{even/odd}}(\omega) = C_{e/o}(E_0) \times \Im F^R_{\text{odd/even}}(\omega)$$

Shiba bound state:

$$E_0 = \Delta \frac{1 - \alpha^2 + \beta^2}{\sqrt{(1-\alpha^2+\beta^2)^2 + 4\alpha^2}}$$

$$\alpha = \pi\nu_0 J$$
$$\beta = \pi\nu_0 V$$

$$C_e(E_0) = -\frac{2}{\Delta}[E_0 + \pi J \nu_0 \sqrt{\Delta^2 - E_0^2}]$$
$$= -\frac{2}{\pi} \frac{1 + \beta^2 + \alpha^2}{\sqrt{(1-\alpha^2+\beta^2)^2 + 4\alpha^2}}$$

Concrete protocol to extract the odd-ω pairing

Assuming a constant DOS in the normal regime

$$\hat{G}(\omega) = \frac{1}{\omega + i\eta - E_0} \begin{bmatrix} u^2 & uv \\ uv & v^2 \end{bmatrix} \qquad u^2, v^2 = 2\pi\alpha\nu_0\Delta \frac{1 + (\alpha \pm \beta)^2}{((1 - \alpha^2 + \beta^2)^2 + 4\alpha^2)^{3/2}}$$

$$\Rightarrow \quad \rho(\omega) = \frac{\eta u^2/\pi}{(\omega - E_0)^2 + \eta^2} + \frac{\eta v^2/\pi}{(\omega + E_0)^2 + \eta^2}$$

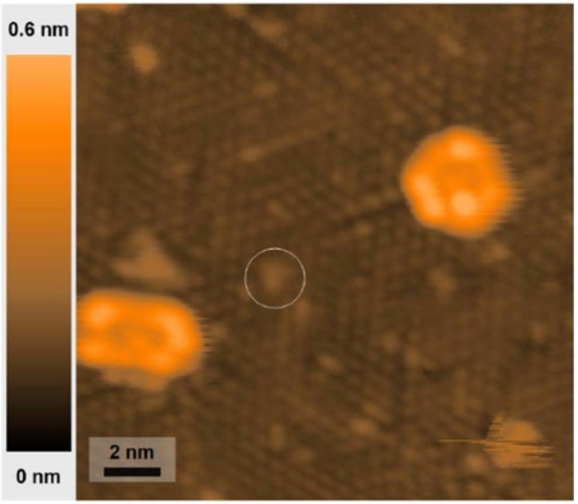
M. Ruby et al., Phys. Rev. Lett. 115, 087001(2015)

$$\Rightarrow \quad C_e(E_0) = -\frac{u^2 + v^2}{\pi u v}$$

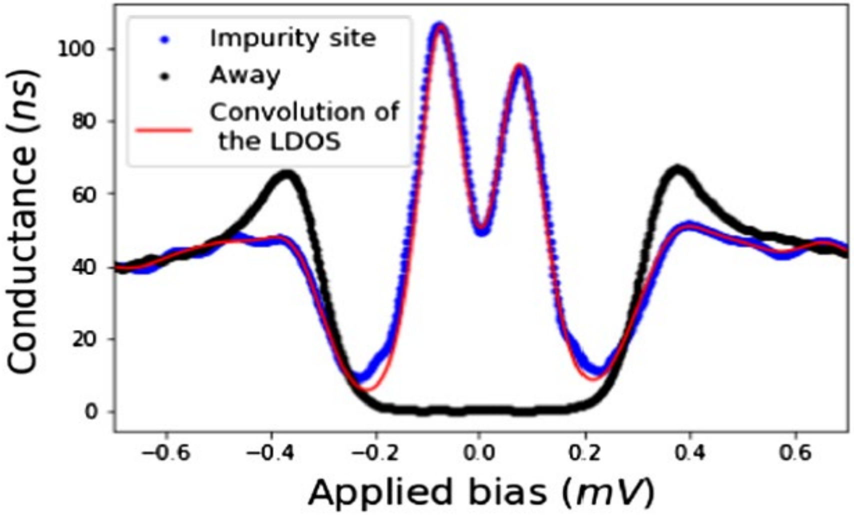
$E_0, u, v, \eta,$ **funtions of** $J, V, \Delta \ldots$ ⇒ Extracted from the measured deconvoluted LDoS

$$\Im F^R_{odd}(\omega) \; = \; \rho_{even}(\omega)/C_e(E_0)$$

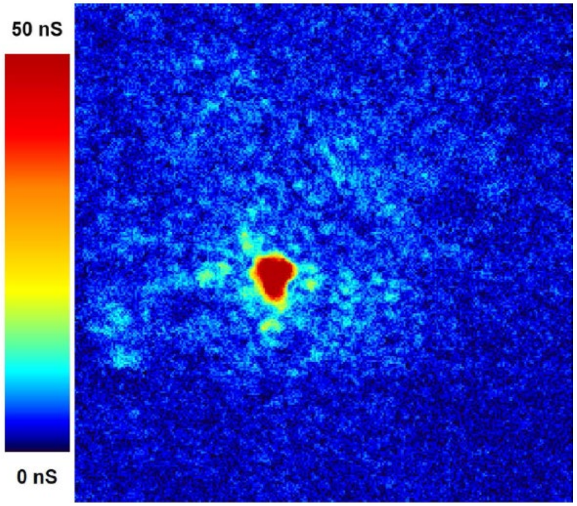
Odd-Frequency Pairing on the impurity site



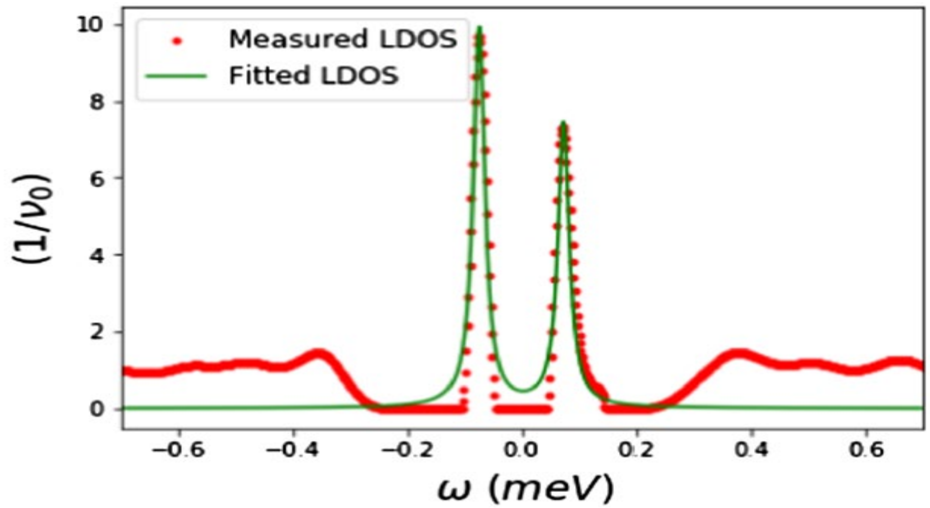
Pb/Si(111) monolayer



Conductance on top of the impurity



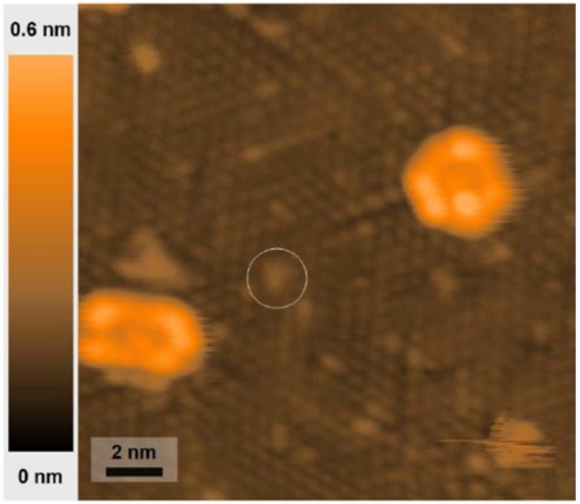
Conductance map at E_F



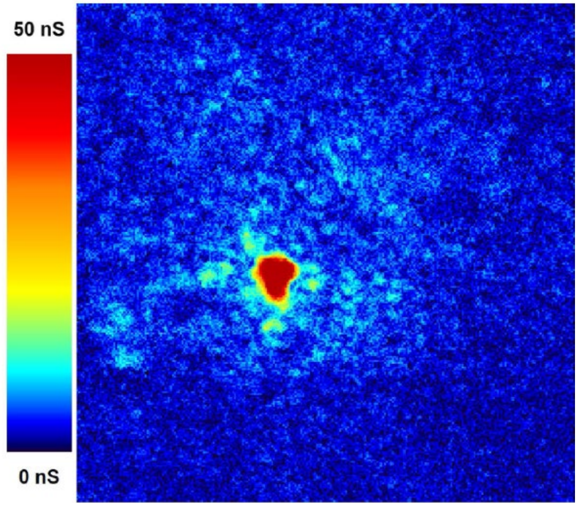
Deconvoluted LDOS on top of the impurity

V. Perrin et al., Phys. Rev. Lett. 125, 117003 (2020)

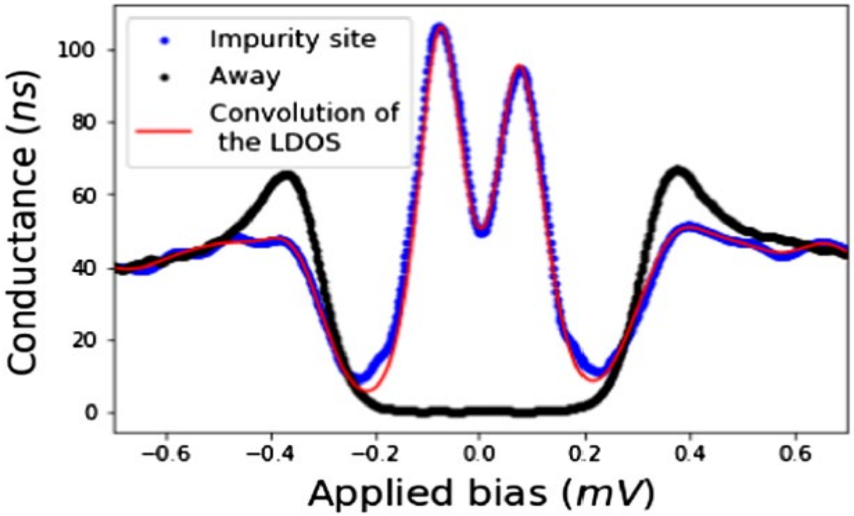
Odd-Frequency Pairing on the impurity site



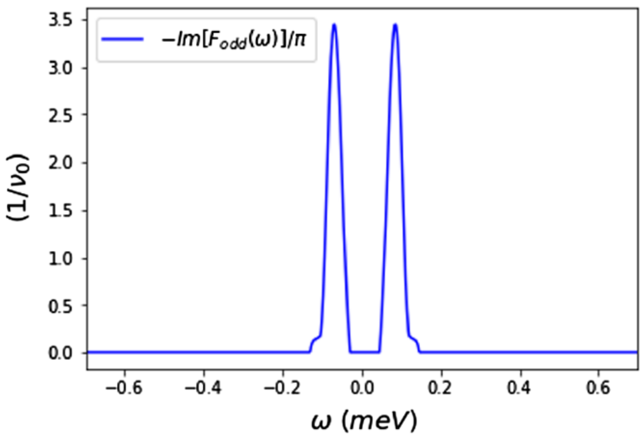
Pb/Si(111) monolayer



Conductance map at E_F



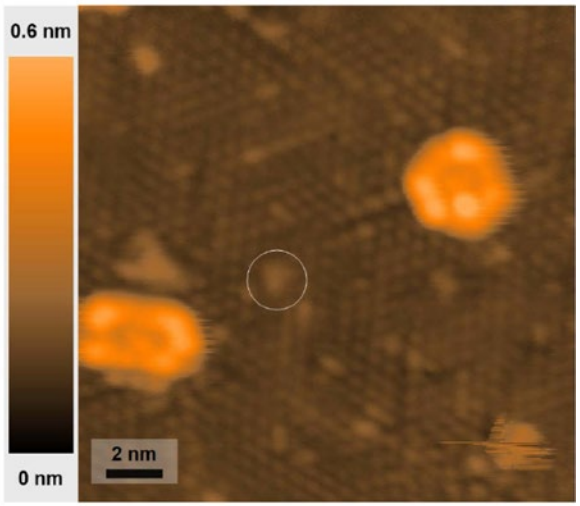
Conductance on top of the impurity



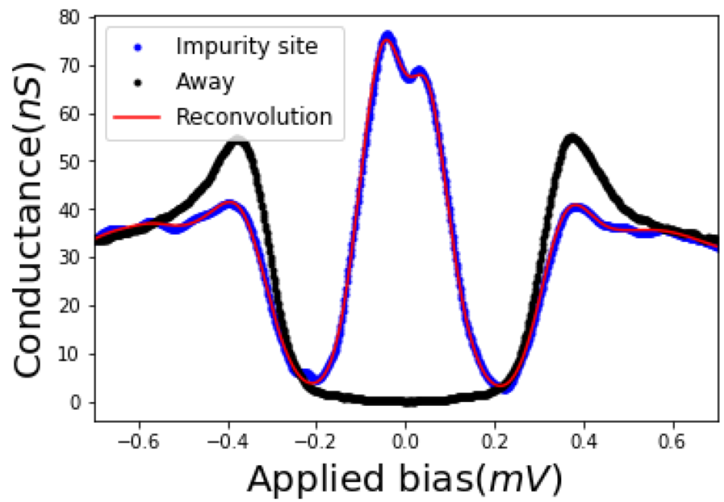
Odd-triplet correlations on top of the impurity

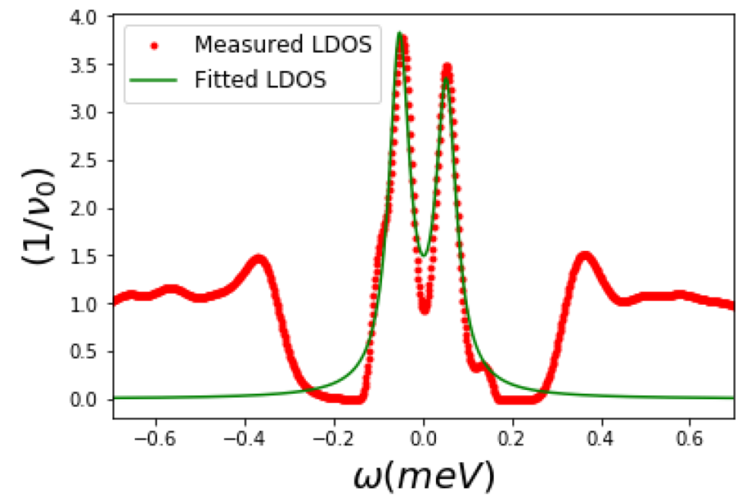
V. Perrin et al., Phys. Rev. Lett. 125, 117003 (2020)

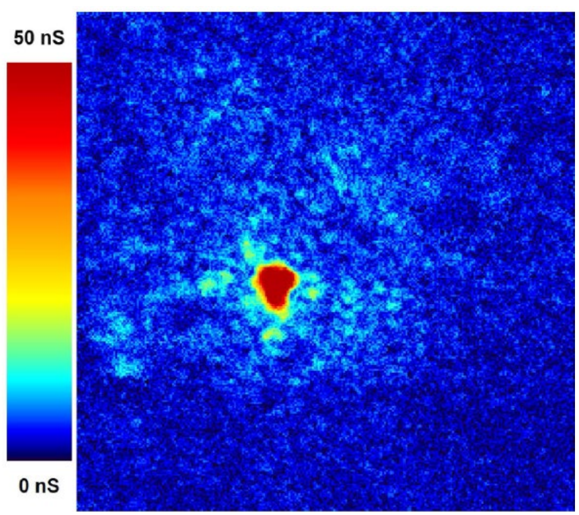
Another magnetic impurity



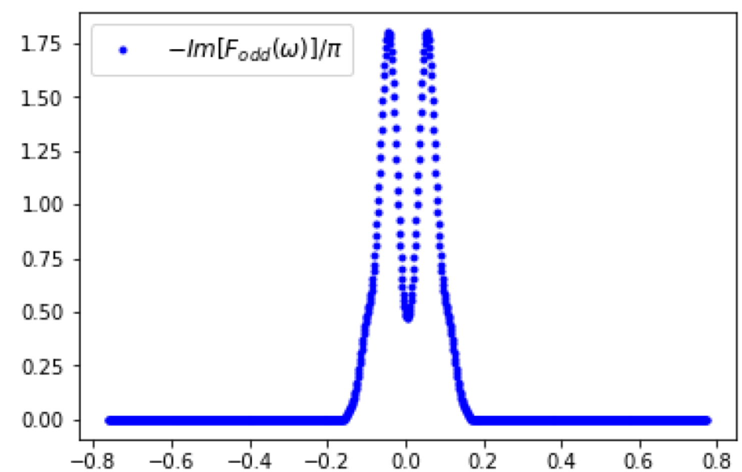
Pb/Si(111) monolayer







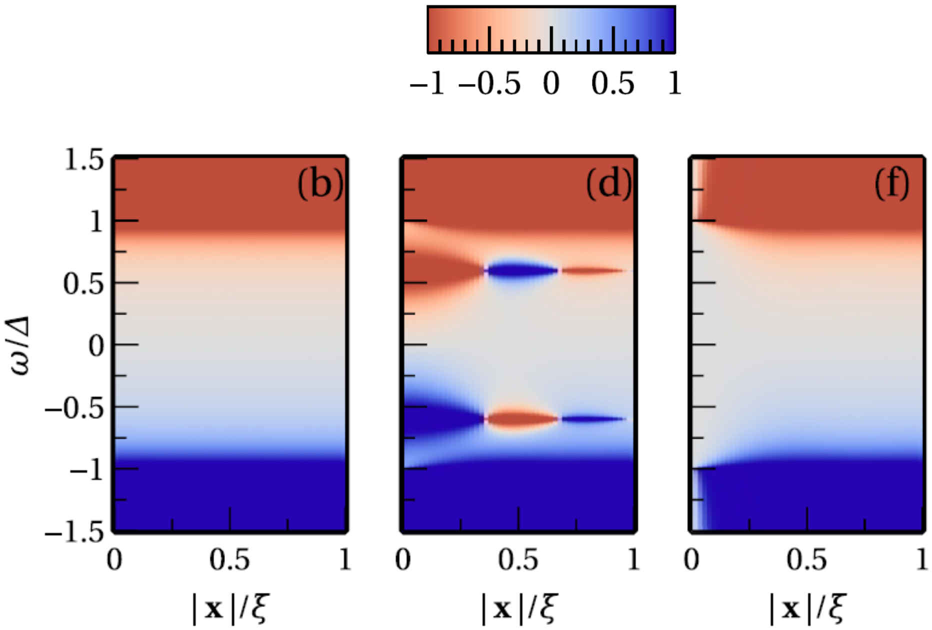
Conductance map at E_F



A macroscopic fraction of the LDOS !

V. Perrin et al., Phys. Rev. Lett. 125, 117003 (2020)

Space dependence of odd-ω pairing

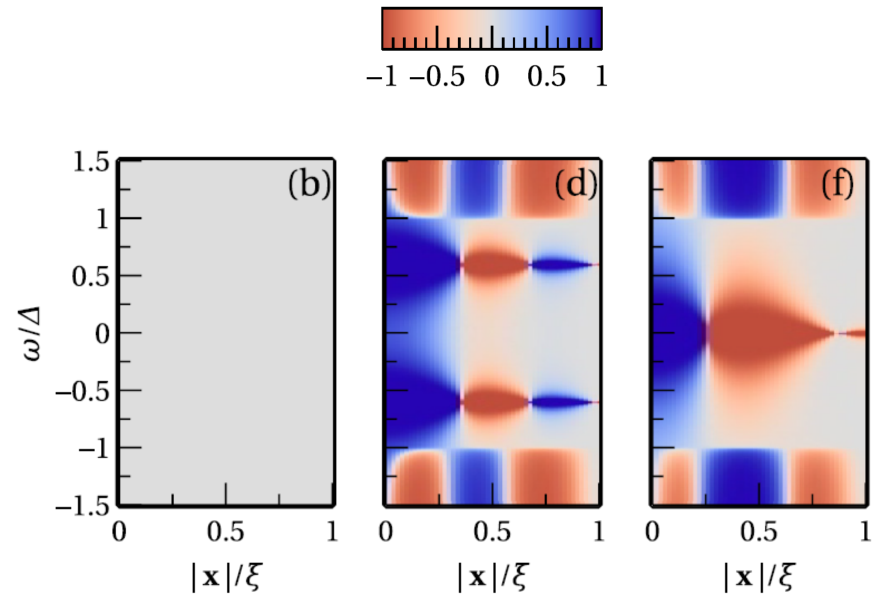


Even-singlet correlations

b) No impurity

d) Impurity with E_0 = 0.6 D

c) Impurity with E_0 = 0



Odd-triplet correlations

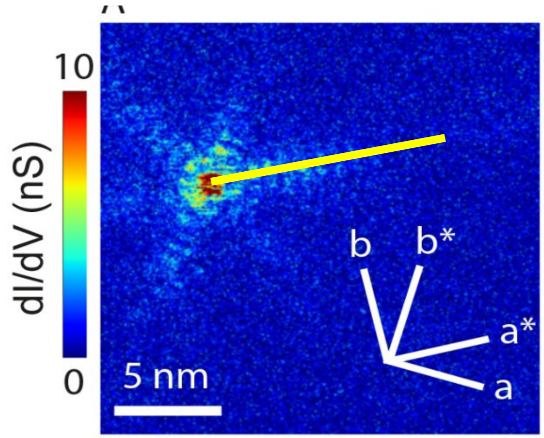
b) No impurity

d) Impurity with E_0 = 0.6 D

c) Impurity with E_0 = 0

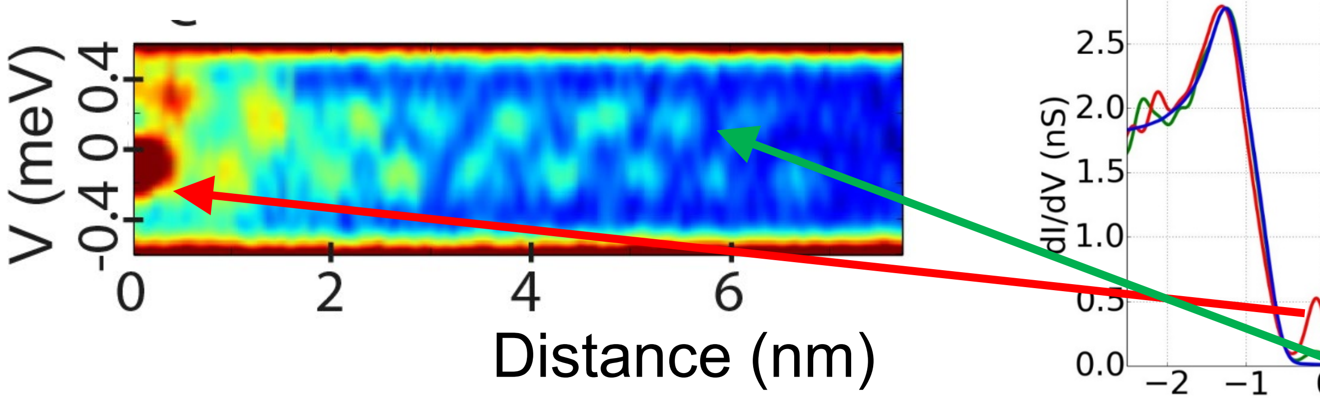
Odd-frequency superconductivity near a magnetic impurity in a conventional superconductor,
D. Kuzmanovski, R. S. Souto and A. V. Balatsky, Phys. Rev. B 101, 094505 (2020)

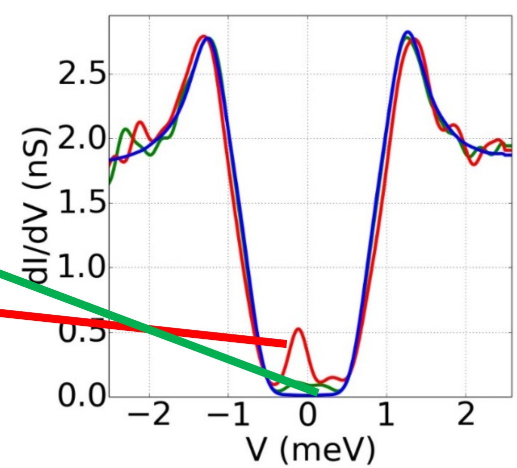
Spatial oscillation of Shiba bound states
Electron-hole asymmetry



•Oscillations of the local density of states with a phase opposition between positive and negative energy states

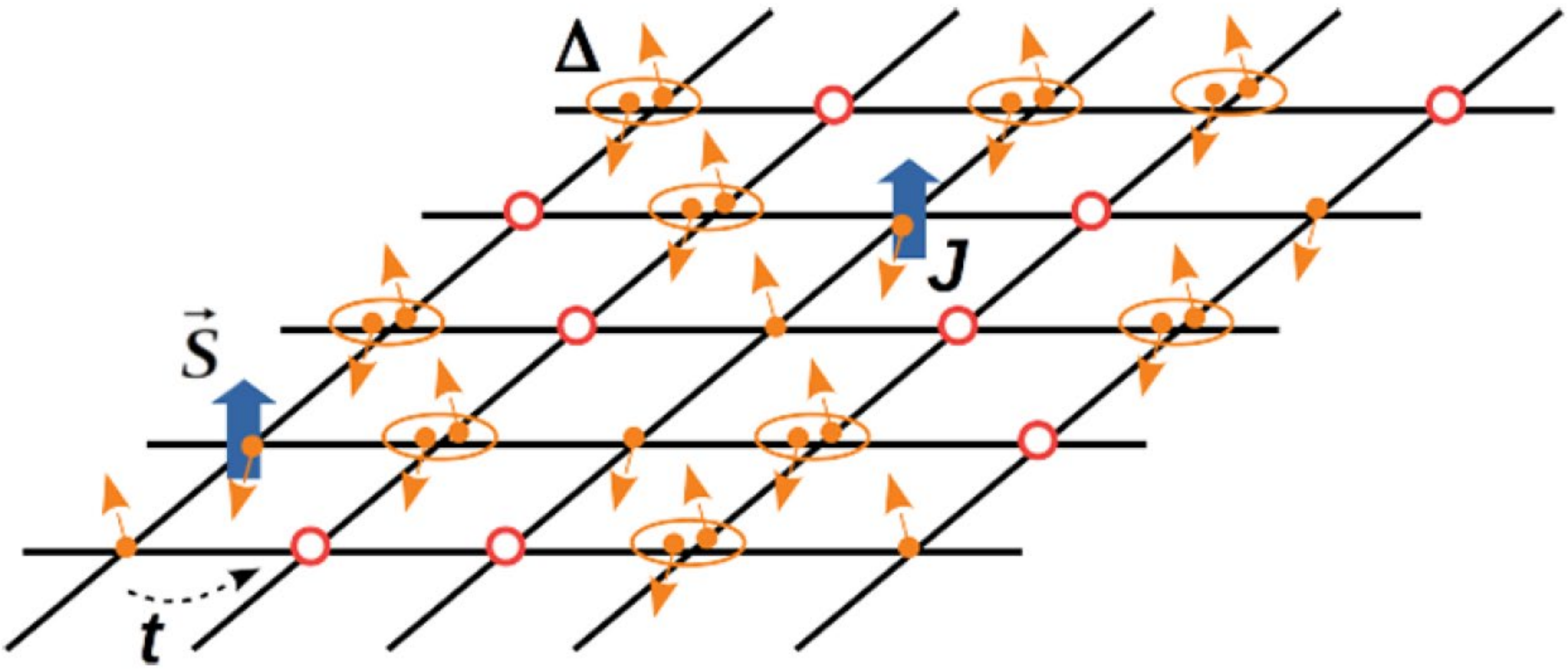
•Decrease of the Shiba bound states on a size of the order of the coherence length ξ



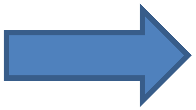


G. Ménard et al., Nature Physics 11, 1013 (2015)

A dilute magnetic s-wave superconductor



a superconductor with a finite concentration, x, of magnetic impurities



Magnetic impurities are again treated classically

A DMFT approach

We solve this problem by the **Dynamical Mean Field Theory** (DMFT) approach (exact in the infinite-dimension limit).

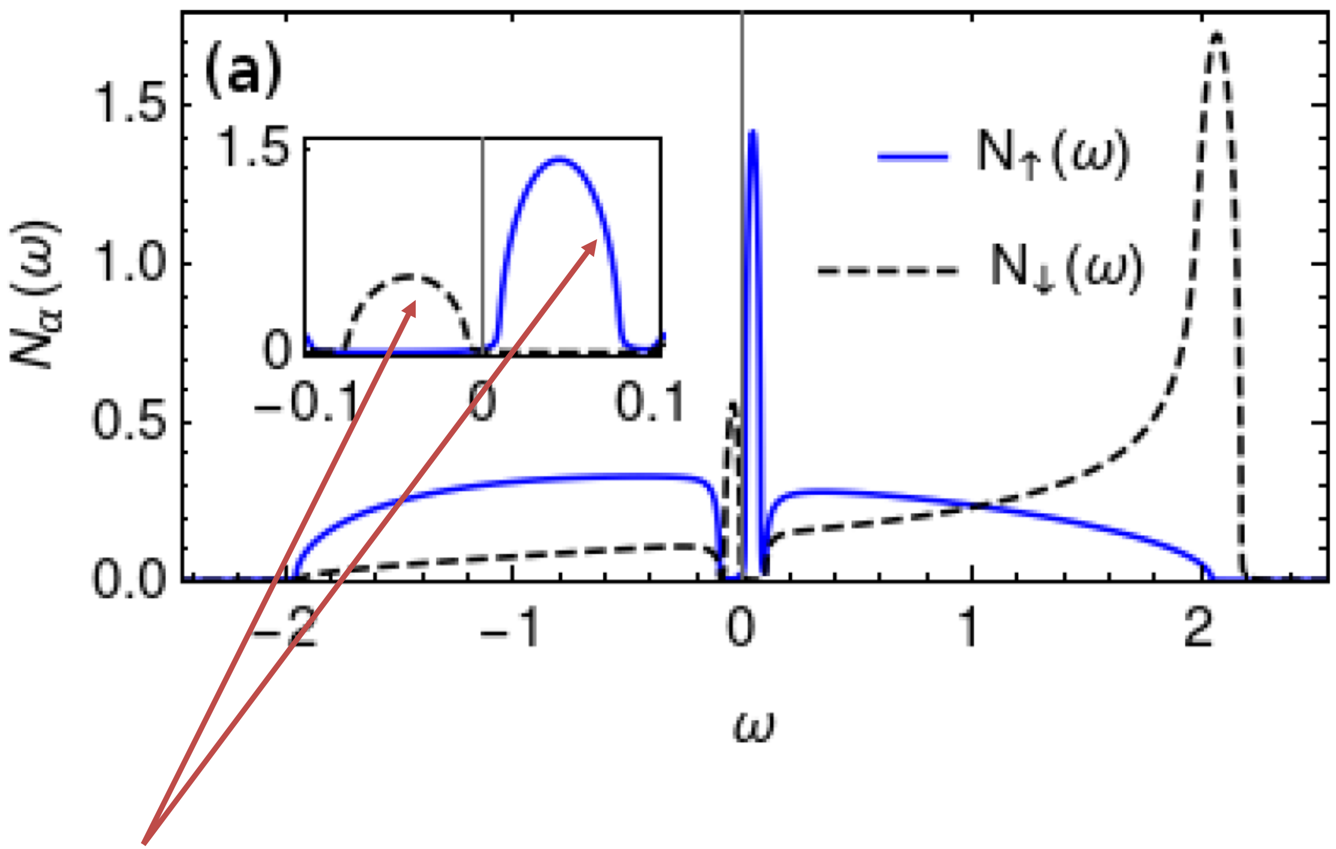
A set of self-consistent equations:

$$\begin{cases} \hat{G}_{nm}^{-1}(i\omega) = i\omega\mathbb{1} + \mu\tau^z - \Delta\tau^x - t^2\tau^z\hat{G}_{av}\tau^z, \\ \hat{G}_{m}^{-1}(i\omega) = i\omega\mathbb{1} + (\mu + \delta_\mu)\tau^z - t^2\tau^z\hat{G}_{av}\tau^z - J\mathbb{1} \\ \text{with} \quad \hat{G}_{av} = x\hat{G}_m + (1-x)\hat{G}_{nm} \end{cases}$$

Shiba impurity bands

We solve this problem by the **Dynamical Mean Field Theory** (DMFT) approach (exact in the infinite-dimension limit).

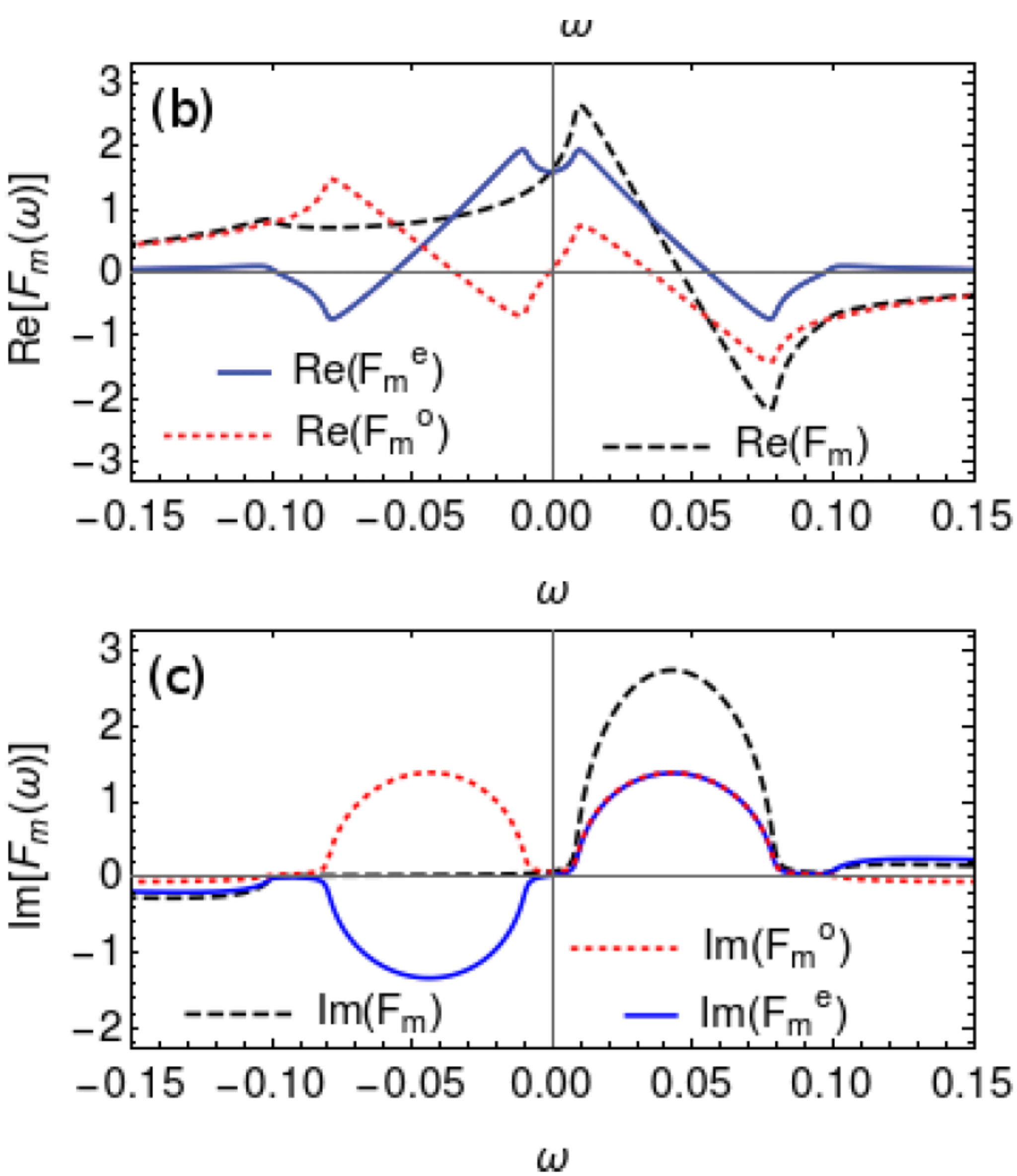
Density of states



Polarized impurity (Shiba) bands

F.L.N. Santos et al., Phys. Rev. Res. 2, 033229 (2020)

Triplet s-wave odd-frequency pairing



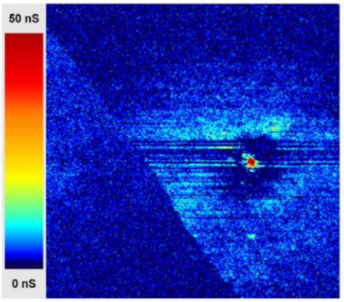
$$\mathrm{Im}[F_m^o(\omega)] = a_F\left[\frac{N_\uparrow(\omega)}{a_\uparrow} + \frac{N_\downarrow(\omega)}{a_\downarrow}\right].$$

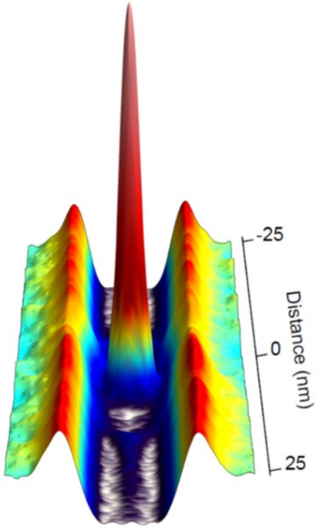
Proportionality relations valid here too!

F.L.N. Santos et al., Phys. Rev. Res. 2, 033229 (2020)

Conclusion

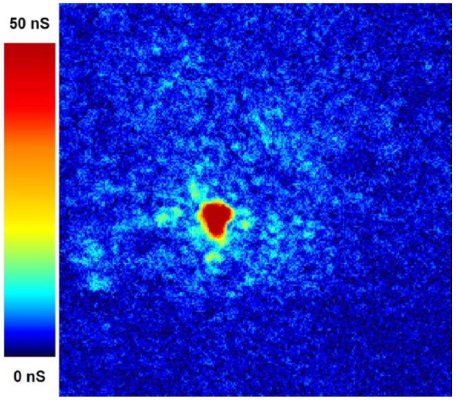
Majorana zero-energy bound states in defect core:
Interpreted with a non-trivial magnetic texture

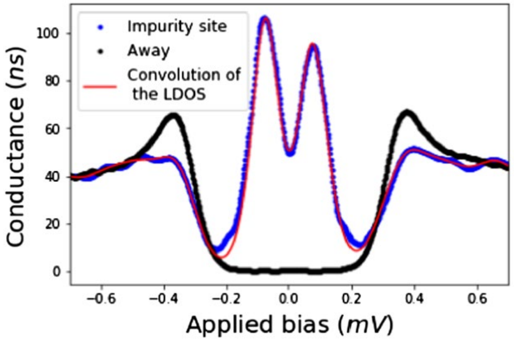




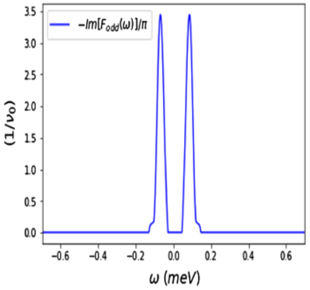
G. Ménard et al, Nature Comm (2019)

Odd-w frequency triplet pairing around a magnetic impurity





Conductance on top of the impurity



Odd-triplet correlations on top of the impurity

V. Perrin et al., Phys. Rev. Lett. 125, 117003 (2020)

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Thanks for your attention !