«Magnetic impurities in superconductors: Role of many-body interactions »

Pascal Simon
University Paris Saclay

opology and Geometry Beyond Perfect Crystals, Stockholm, 28-05-25

Main Collaborators

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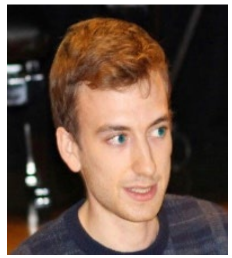
- Mateo Uldemolins
- Vivien Perrin
- Andrej Mesaros



IMN Nantes

- Laurent Cario

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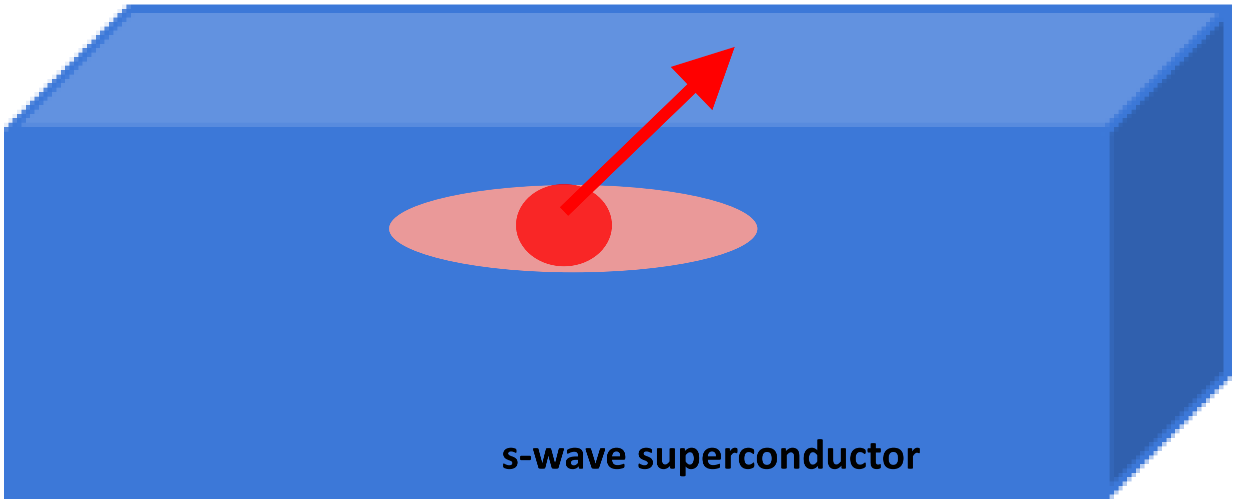
- F. Massee
- M. Aprili
- A. Palacio-Morales




Genda Gu Brookhaven National Laboratory

Why studying magnetic impurities in a superconductor ?

An old solved problem ?



Magnetic adatom: pair-breaking defect

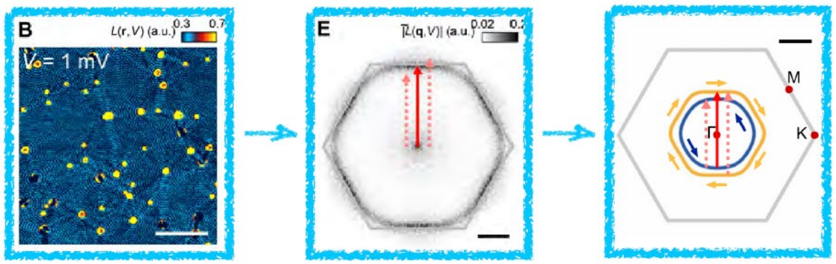
In-gap excitation localized on the impurity: **Yu-Shiba-Rusinov (YSR) bound states**

Yu, Act. Phys. Sin. 21, 75 (1965), Shiba, Pr. Th. Phys. 40, 435 (1968), Rusinov, Sov. JETP 9, 85 (1969).

Motivation 1: Local defects as probing tools

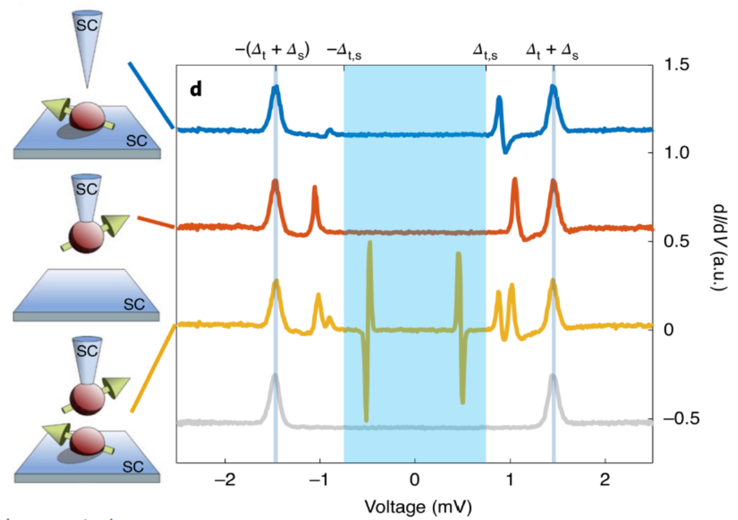
Quasiparticle Interference (QPI)

Real space — q-space (FT) — Band structure



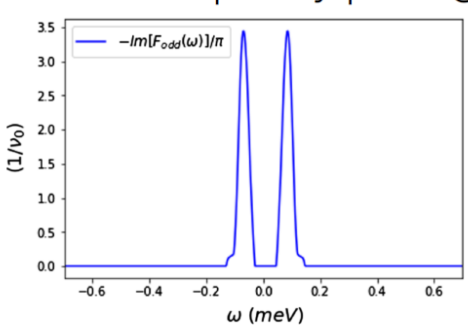
Yim et al. Sci. Adv. 7 eabd7361 (2021)

YSR-state functionalized tips



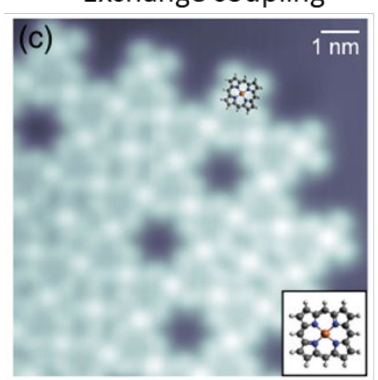
Huang et al.
Nat. Phys. 16, 1227-1231 (2020)

Odd-frequency pairing



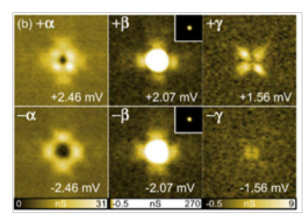
Perrin et al.
PRL 125, 117003 (2020)

Exchange coupling



L.Farinacci et al.
PRL 121, 196803(2018)

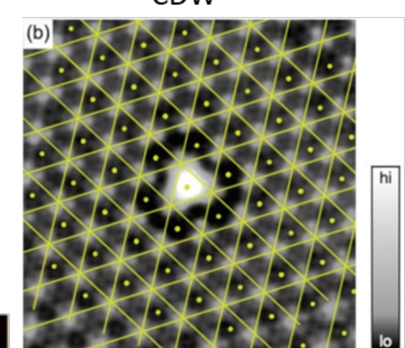
Orbitals



M.Ruby et al.
PRL 117,186801 (2016)

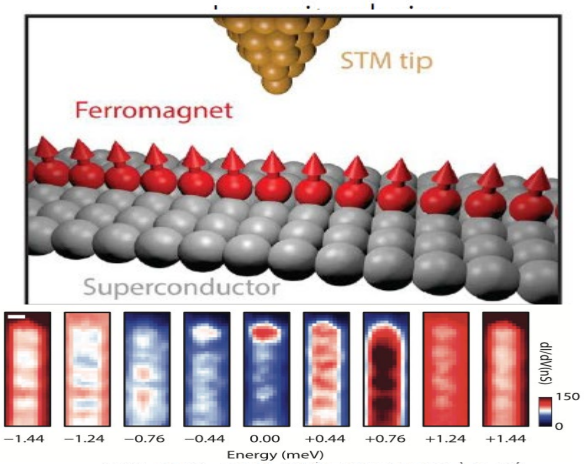
D.J.Choi et al.
Nat.Comm. 8 15175(2017)

CDW



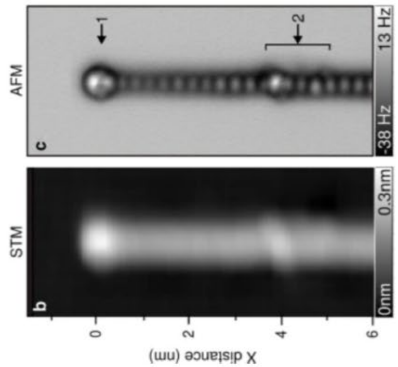
E.Liebhaber et al.
Nano. Lett. 20, 339(2020)

Motivation 2: Engineering exotic states



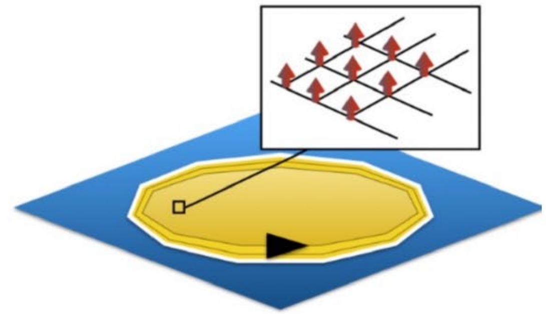
S. Nadj-Perge et al., Science **346,** 6209 (2014)

Majorana states



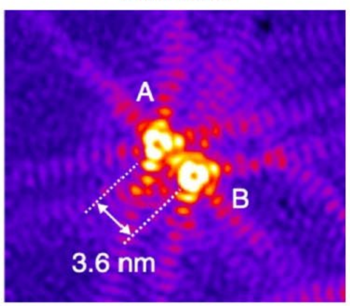
Pawlak et al. npj Q. Info 2, 16035 (2016)

Impurity lattices for topological SC

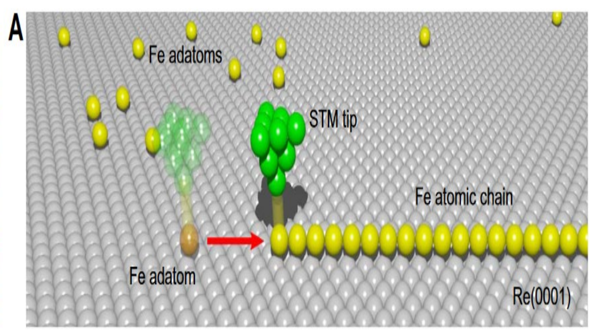


Rontynen, Ojanen. PRB 93, 094521 (2016)

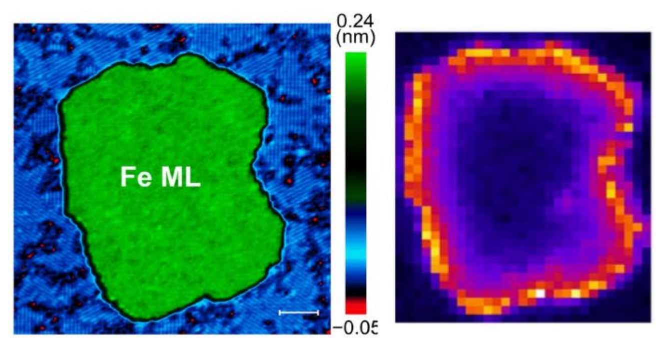
Dimers



Kim et al. Nat. Comm. 11, 4573 (2020)

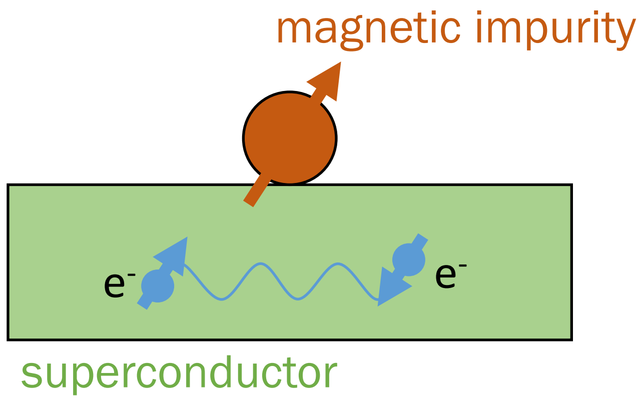


Kim et al. Sci. Adv., **2** eaar5251 (2018)



alacio-Morales et al. Sci. Adv. 5, eaav6600 (2019)

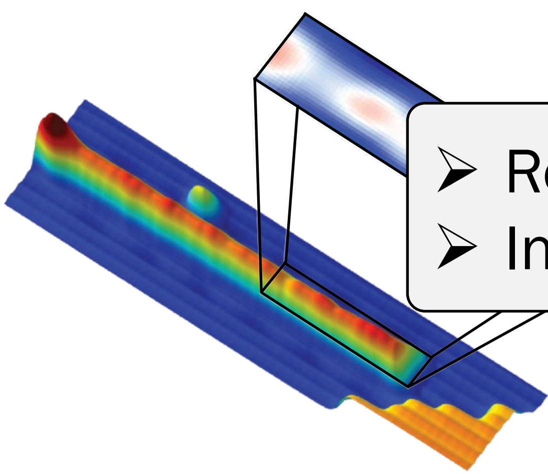
Questions ?



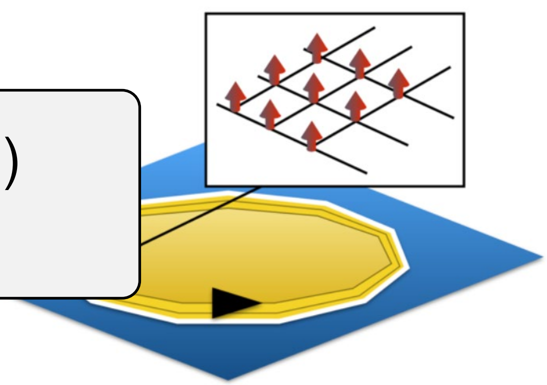
- As a probe of bulk properties
- As a building block

Chains & ladders:
Majorana end states

2D lattices:
Topological superconductivity



- Relaxation (lifetime)
- Interactions



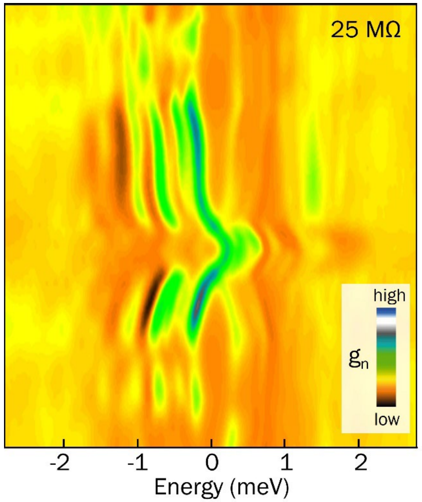
PRB **93**, 094521 (2016)

Review: Jäck, Xie, Yazdani, Nature Physics (2021)

Today's menu

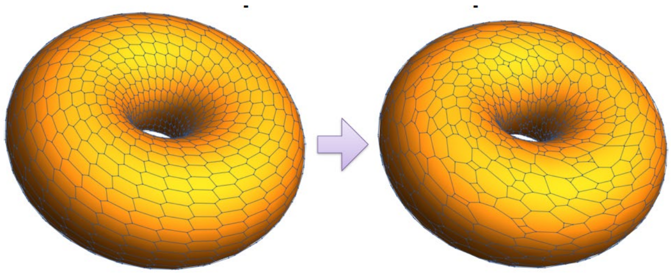
1. Multi-channel quantum phase transition

M. Uldemolins et al., Nature Comm 15, 8526 (2024)



2. Crystalline band topology apllied to amorphous counter part

by Andrii Sirota



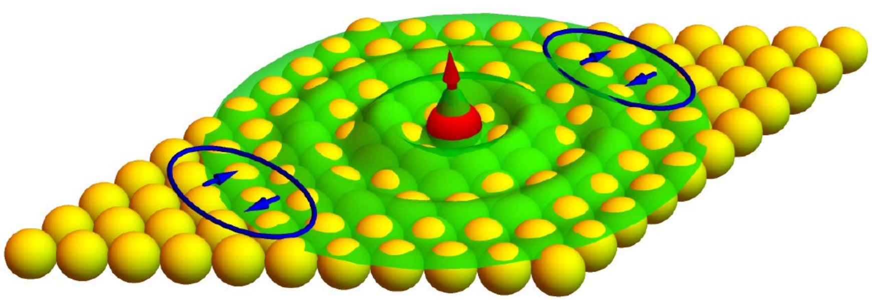
A magnetic impurity in a superconductor

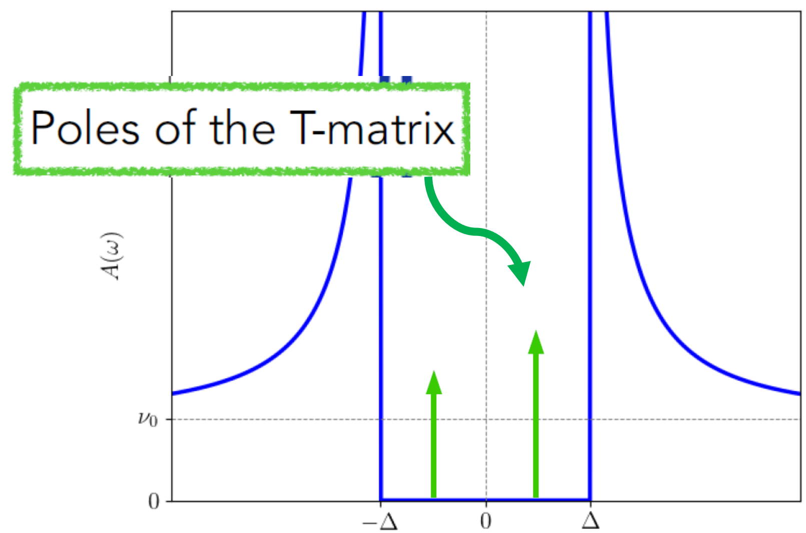
$$H = \sum_{\mathbf{k}\sigma} \xi_k c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \Delta \sum_{\mathbf{k}} \left(c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \right) - J\left(c^\dagger_{0\uparrow} c_{0\uparrow} - c^\dagger_{0\downarrow} c_{0\downarrow} \right) + K\left(c^\dagger_{0\uparrow} c_{0\uparrow} + c^\dagger_{0\downarrow} c_{0\downarrow} \right)$$

Assumes Δ constant
(homogeneous))

Assumptions about the impurity

- Local and isotropic
- Classical spin
- SC gap not affected locally



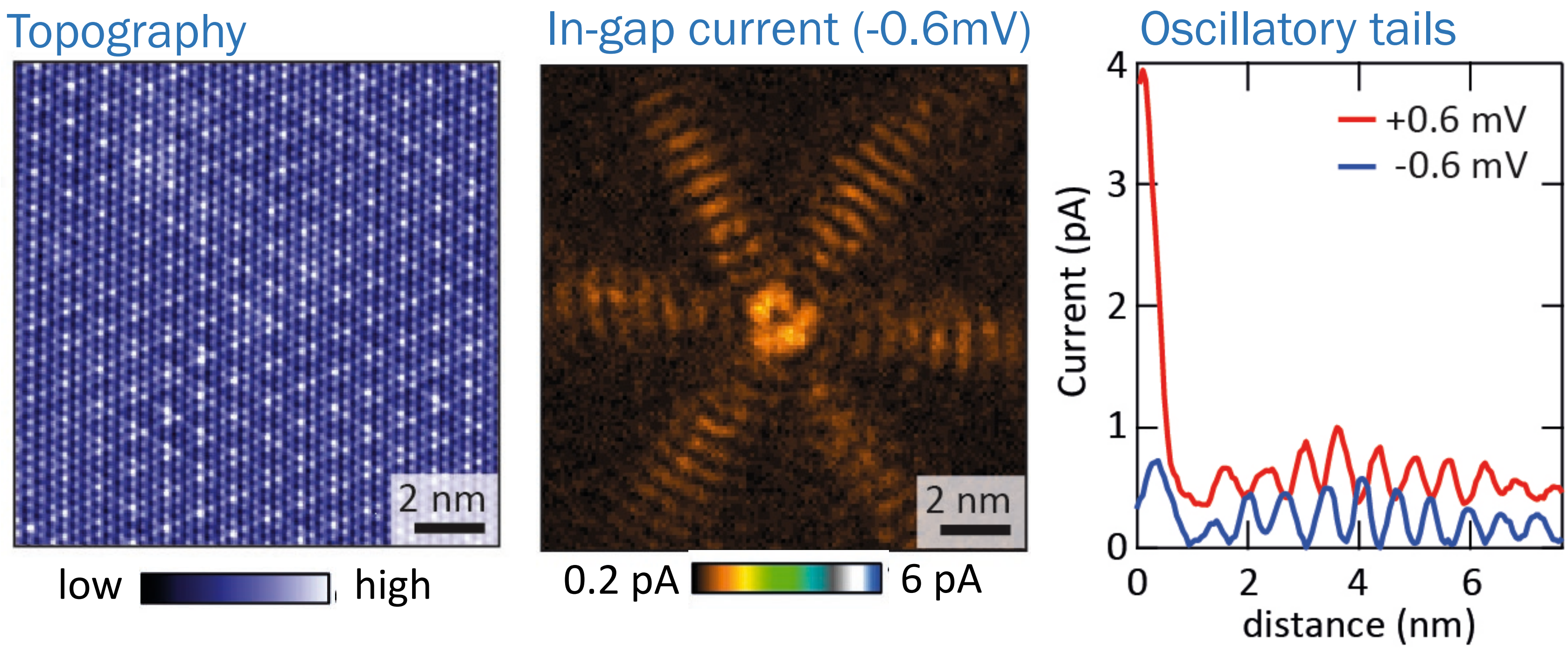


YSR (K=0)

$$E_0 = \Delta \frac{1-\alpha^2}{1+\alpha^2} \qquad \alpha = \pi \nu_0 J S$$

Yu Lu (1965), Shiba (1968),Rusinov (1969)

Extended YSR in NbSe2



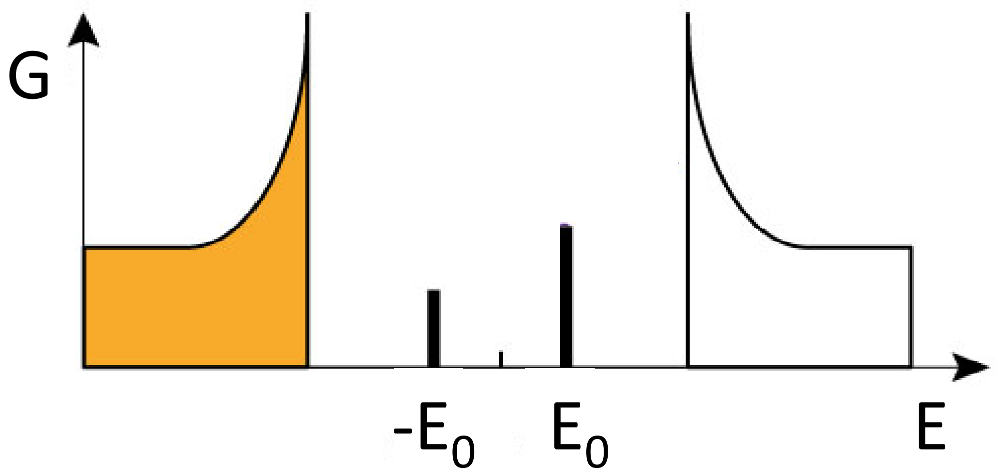
U. Thupakula et al., Phys. Rev. Lett. **128**, 247001 (2022)

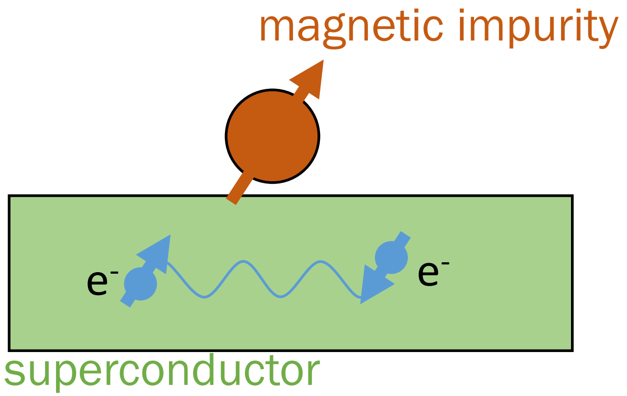
see also Ménard et al., *Nat. Phys.* **11**, 1013 (2015)

Remark: one can qualitatively and quantitatively understand the precise shape of the bound state and relate it to the Fermi surface anisotropy:

See M Uldemolins, A Mesaros, PS, Phys. Rev. B 105, 144503 (2022);
& M Uldemolins, F Massee, T Cren, A Mesaros, PS, Phys Rev. B 110, 224519 (2024).

Lifetime of Yu-Shiba-Rusinov (YSR) states ?



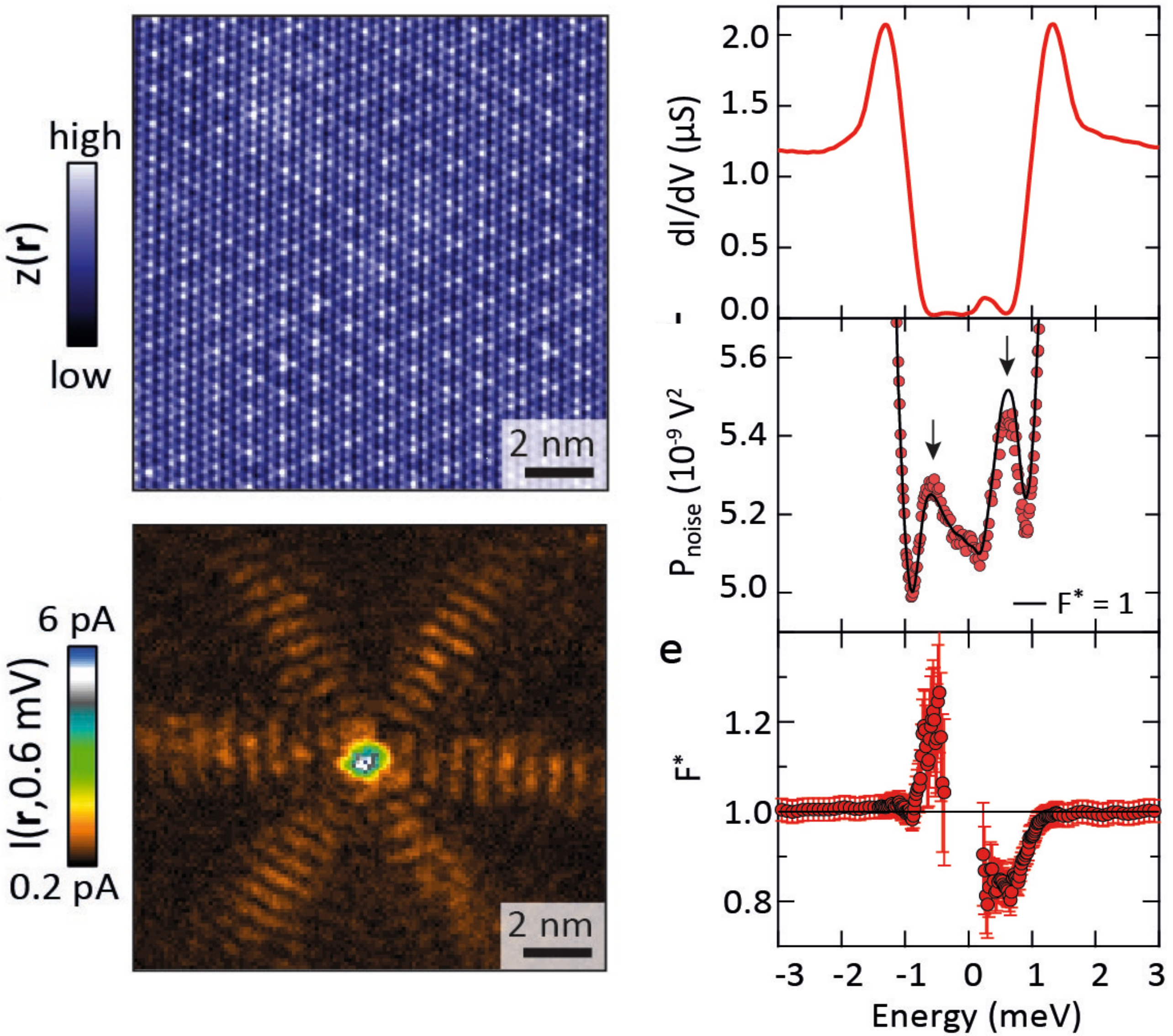


Science **275**, 1767 (1997)
PRL **100**, 2268 (2008)
Nat. Phys. **11**, 1013 (2015)
PRL **115**, 087001 (2015)
...
Reviews:
Rev. Mod. Phys. **78**, 373 (2006)
Prog. Surf. Sci. **93**, 1-19 (2018)

Lifetime: intrinsic width $\ll 3.5k_BT$

How can we extract it ?

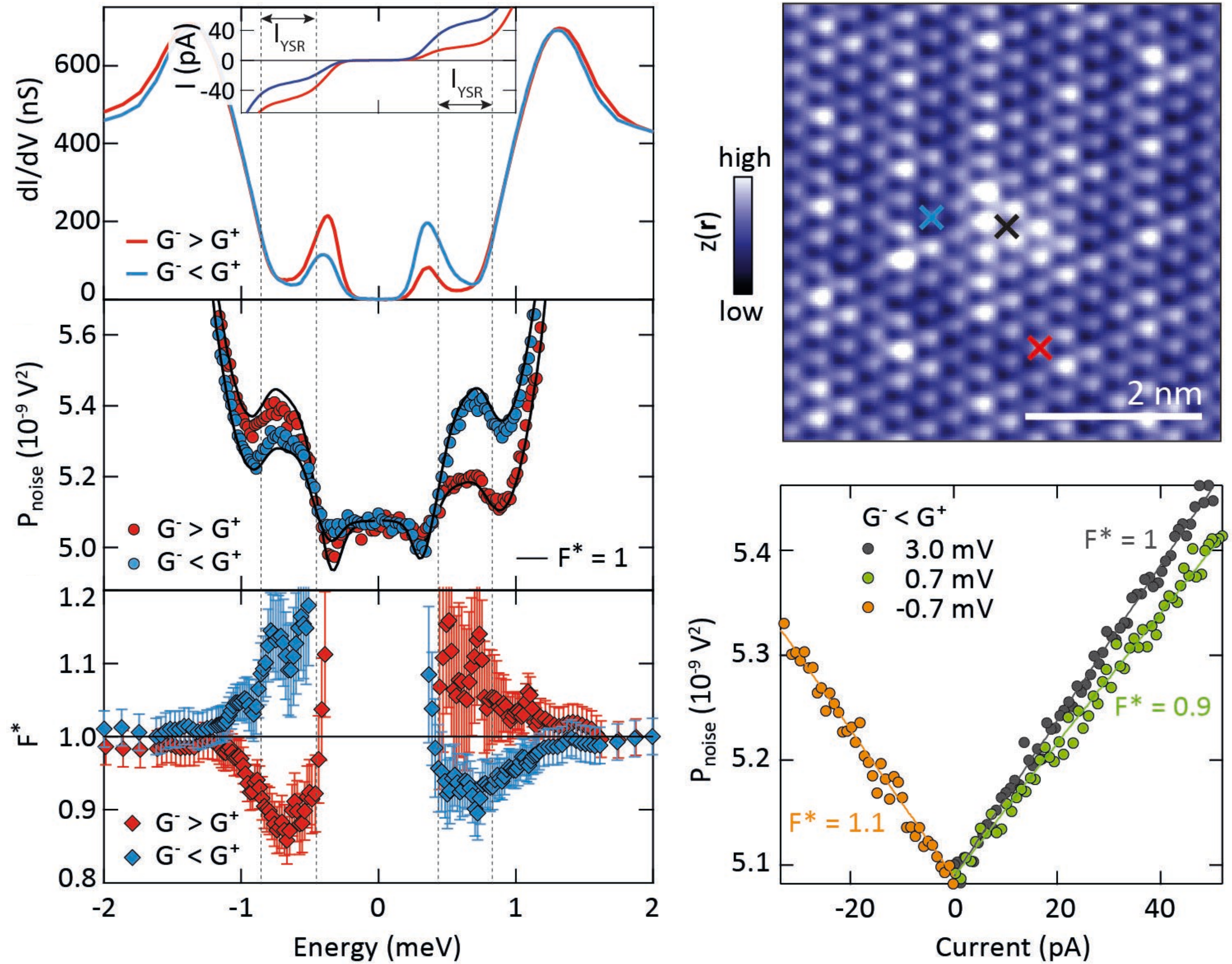
Noise tomography of YSR states in 2H-$NbSe_2$



- Big peak: noise reduced
- Small peak: noise enhanced

U. Thupakula et al., PRL (2022)

Noise tomography of YSR states in 2H-$NbSe_2$



U. Thupakula et al., PRL (2022)

A simple theoretical model

Assumptions :

- Retain only YSR contributions to the transport observables
- Local tunneling of quasiparticles from tip to sample.
- Neglect direct injection of quasiparticles into the impurity's orbitals.

→ Expected to be relevant to describe STM experiments probing the tail of the YSR.

$$\mathcal{H} = \int \frac{d\mathbf{k}}{(2\pi)^d} \psi_T^\dagger(\mathbf{k}) \epsilon_T(\mathbf{k}) \tau_z \psi_T(\mathbf{k}) + \int \frac{d\mathbf{k}}{(2\pi)^d} \psi_S^\dagger(\mathbf{k}) [\epsilon_S(\mathbf{k}) \tau_z + \Delta \tau_x] \psi_S(\mathbf{k})$$

metallic tip — superconducting substrate

$$+\psi_S^\dagger(\mathbf{0})(U\tau_z - J)\psi_S(\mathbf{0}) \; + \tilde{t}\{\psi_S^\dagger(\mathbf{r}_0)\tau_z\psi_T + \psi_T^\dagger \tau_z \psi_S(\mathbf{r}_0)\}$$

Classical magnetic impurity — tip-substrate tunnelling

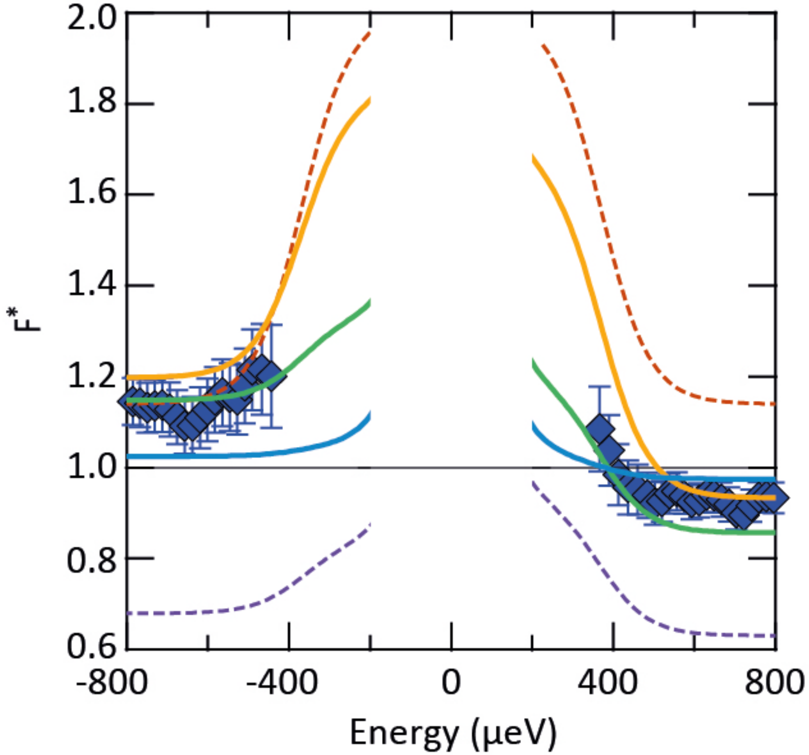
using model from *PRL* **115**, 087001 (2015)

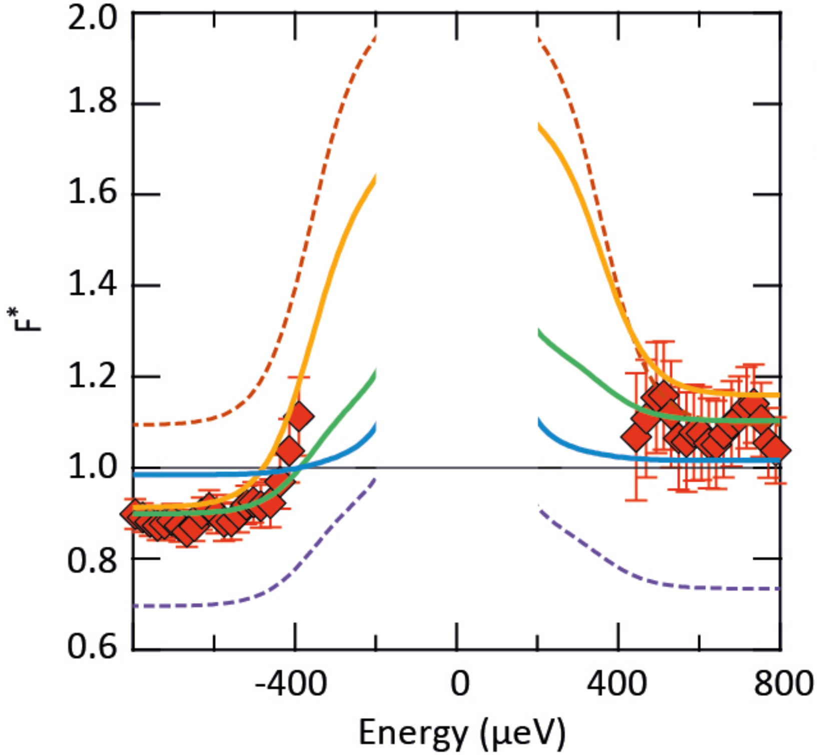
$\Gamma_e \equiv \Gamma u^2, \Gamma_h \equiv \Gamma v^2$ and $\Gamma_t \equiv \Lambda + \Gamma_e + \Gamma_h$

intrinsic life-time (Λ)

all parameters from experiment except Λ

Comparison experiment-theory





Coherent (Andreev) and incoherent (single electron) tunnelling processes operate simultaneously for a single YSR

Λ = 0.1 μeV

Λ = 1 μeV ← Nanosecond scale!

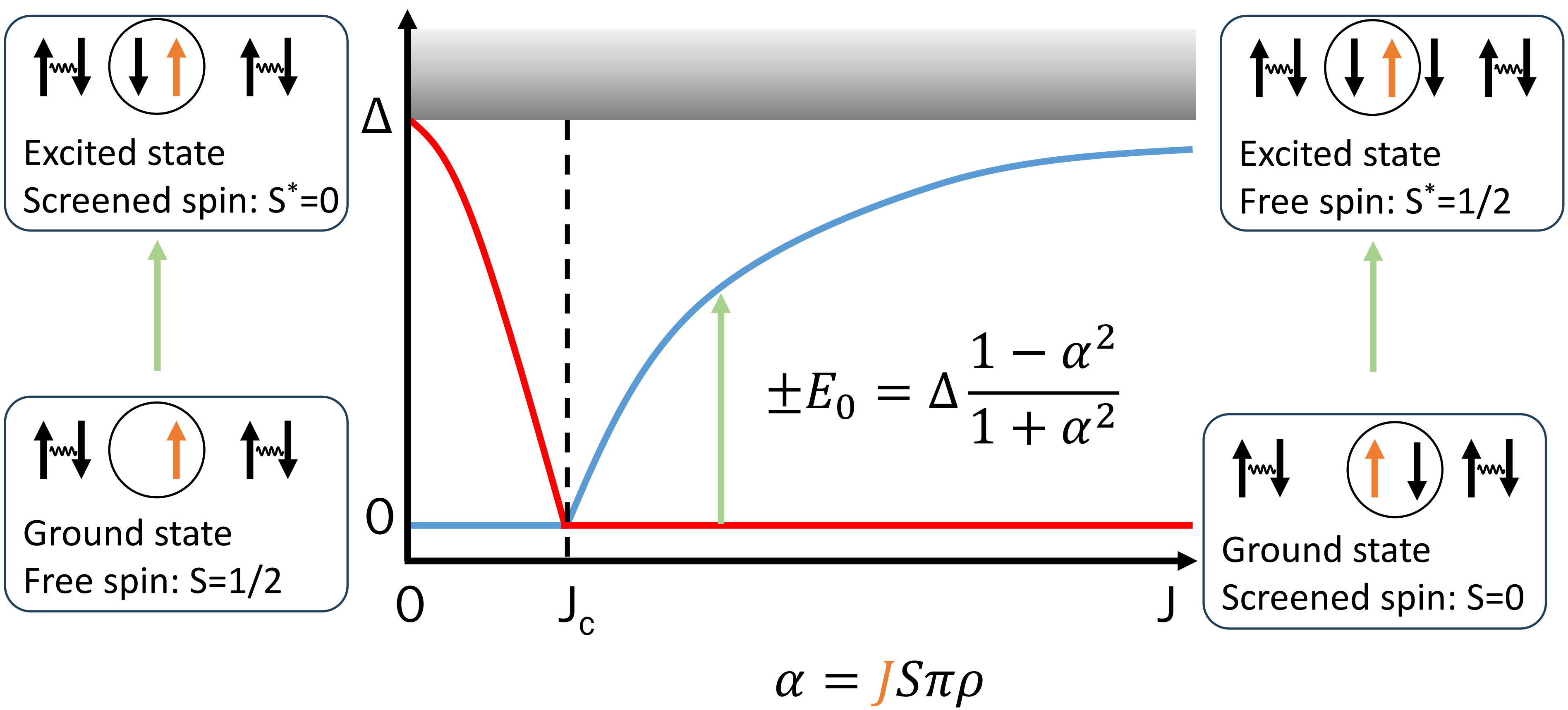
Λ = 10 μeV

$3.5k_BT$ = 200 μeV

U. Thupakula et al., Phys. Rev. Lett. **128**, 247001 (2022)

Quantum phase transition

Excitation spectrum in the YSR
impurity model



Adapted from Franke group : *PRL* **121**, 196803 (2018) and *Prog. Surf. Sci.* **93**, 1-19 (2018)

Impurity models

Complexity

Classical spin	Quantum spin	Anderson impurity
$V_{\text{imp}}^{\text{mag}} = -J \sum_{\sigma,\sigma'} c^{\dagger}_{\mathbf{r}_0,\sigma} \left(\hat{\mathbf{n}} \cdot \sigma\right)_{\sigma,\sigma'} c_{\mathbf{r}_0,\sigma'}$	$H_{\text{s-d}} = -J\,\mathbf{S} \cdot \sum_{\alpha,\alpha'} c^{\dagger}_{\mathbf{r}_0,\alpha} \sigma_{\alpha,\alpha'} c_{\mathbf{r}_0,\alpha'} + DS_z^2 + E(S_x^2 - S_y^2)$	$H_{\text{AI}} = \varepsilon\, n_d + U\, n_{d,\uparrow} n_{d,\downarrow} + V \sum_{k,\sigma} c^{\dagger}_{k,\sigma} d_\sigma + \text{h.c.}$

Large S limit or large longitudinal anisotropy *D*

SW transformation in the local-moment regime U≥πΓ

- Spin fluctuations

- Charge and spin fluctuations
- Explicit impurity-substrate coupling

Science **332**, 6032 (2011)
Nature Commun. **6**, 8988 (2015)

Comm. Phys. **3**, 1-9 (2020)
Nature Commun. **12**, 298 (2021)

Impurity models

Complexity

Classical spin

$$V^{\mathrm{mag}}_{\mathrm{imp}} = -J \sum_{\sigma,\sigma'} c^{\dagger}_{\mathbf{r}_0,\sigma} \left(\hat{\mathbf{n}} \cdot \sigma\right)_{\sigma,\sigma'} c_{\mathbf{r}_0,\sigma'}$$

- Captures most observations
- Widely used to describe YSR states
- Multiple YSR states are simply added up

Quantum spin

$$H_{\mathrm{s-d}} = -J\,\mathbf{S} \cdot \sum_{\alpha,\alpha'} c^{\dagger}_{\mathbf{r}_0,\alpha} \sigma_{\alpha,\alpha'} c_{\mathbf{r}_0,\alpha'} + DS_z^2 + E(S_x^2 - S_y^2)$$

r large
nisotropy *D*

- Spin fluctuations

Science **332**, 6032 (2011)
Nature Commun. **6**, 8988 (2015)

Anderson impurity

$$H_{\mathrm{AI}} = \varepsilon\, n_d + U\, n_{d,\uparrow} n_{d,\downarrow} + V \sum_{k,\sigma} c^{\dagger}_{k,\sigma} d_\sigma + \mathrm{h.c.}$$

SW transformation in the local-moment regime U≥πΓ

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Comm. Phys. **3**, 1-9 (2020)
Nature Commun. **12**, 298 (2021)

Impurity models

Complexity

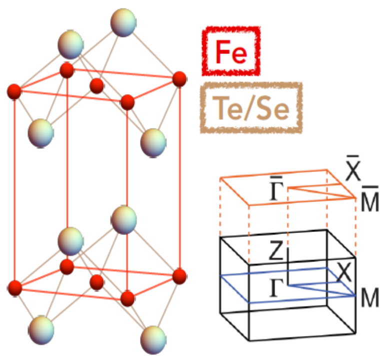
Classical spin

$$V_{\mathrm{imp}}^{\mathrm{mag}} = -J \sum_{\sigma,\sigma'} c_{\mathbf{r}_0,\sigma}^{\dagger} \left(\hat{\mathbf{n}} \cdot \sigma\right)_{\sigma,\sigma'} c_{\mathbf{r}_0,\sigma'}$$

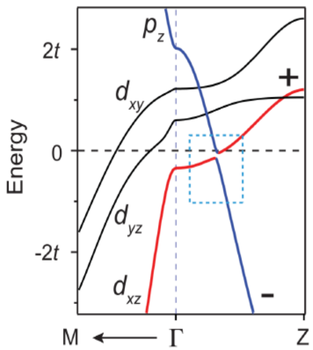
- Captures most observations
- Widely used to describe YSR states
- Multiple YSR states are simply added up

Question: is there an experiment for which classical model does **not** work ?

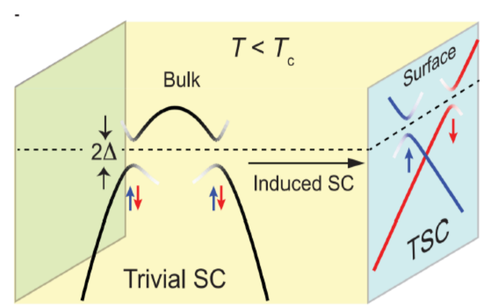
$FeTe_{0.55}Se_{0.45}$: an exotic superconductor in vogue



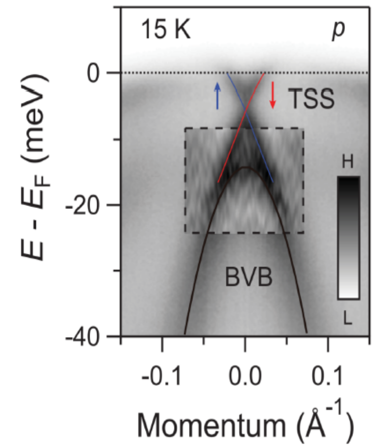
Complex band-structure



Helical Dirac surface states

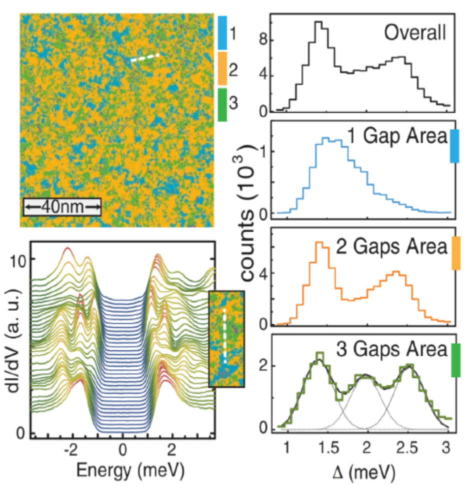


Zhang et al. Sci. 360, 182-186 (2018)



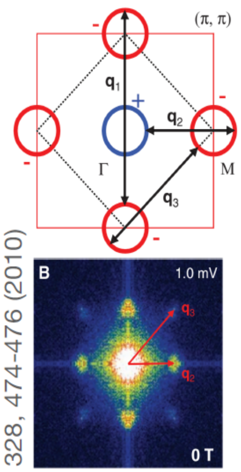
Multi-gap superconductivity

Wang et al. Sci. 367, 104-108 (2020)



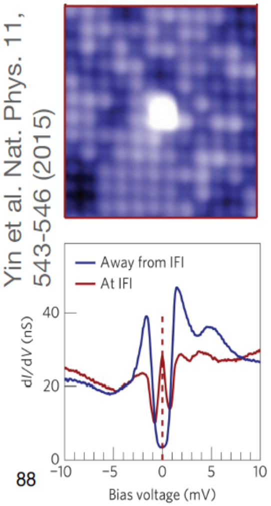
$S_{\pm}$-wave OP ?

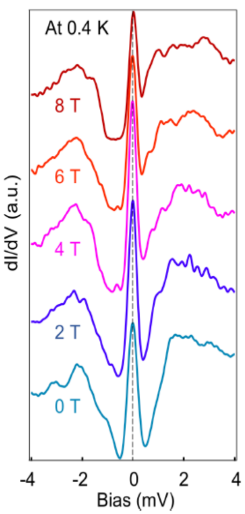
Hanaguri et al. Sci. 328, 474-476 (2010)



Robust zero-bias mode

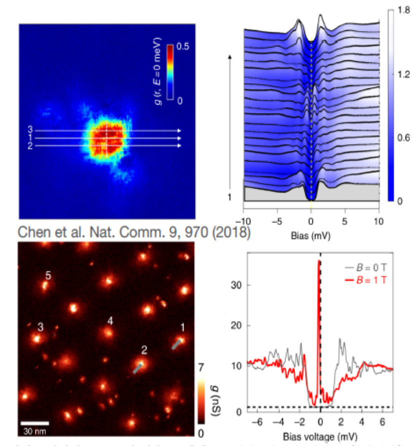
Yin et al. Nat. Phys. 11, 543-546 (2015)





Fan et al. Nat. Comm. 12, 1348 (2021)

Vortex states



Chen et al. Nat. Comm. 9, 970 (2018)

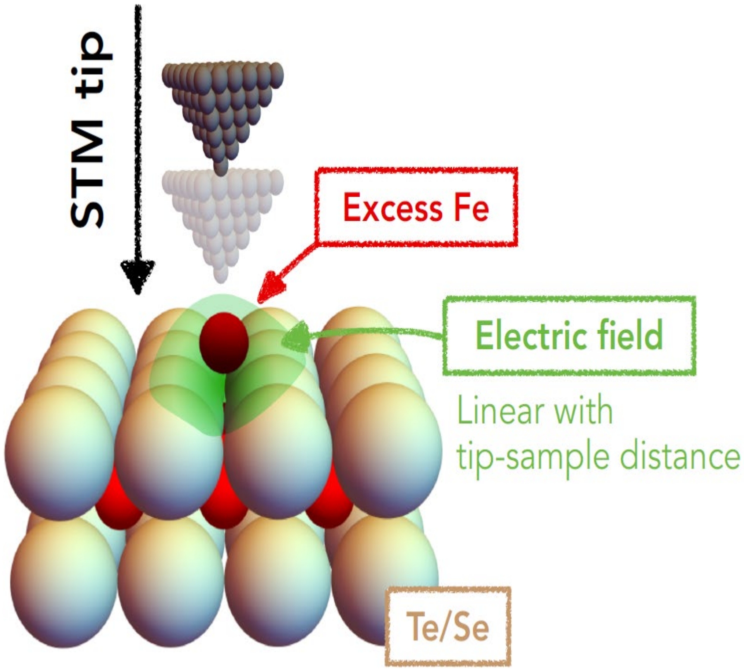
Machida et al. Nat. Mat. 18, 811-815 (2019)

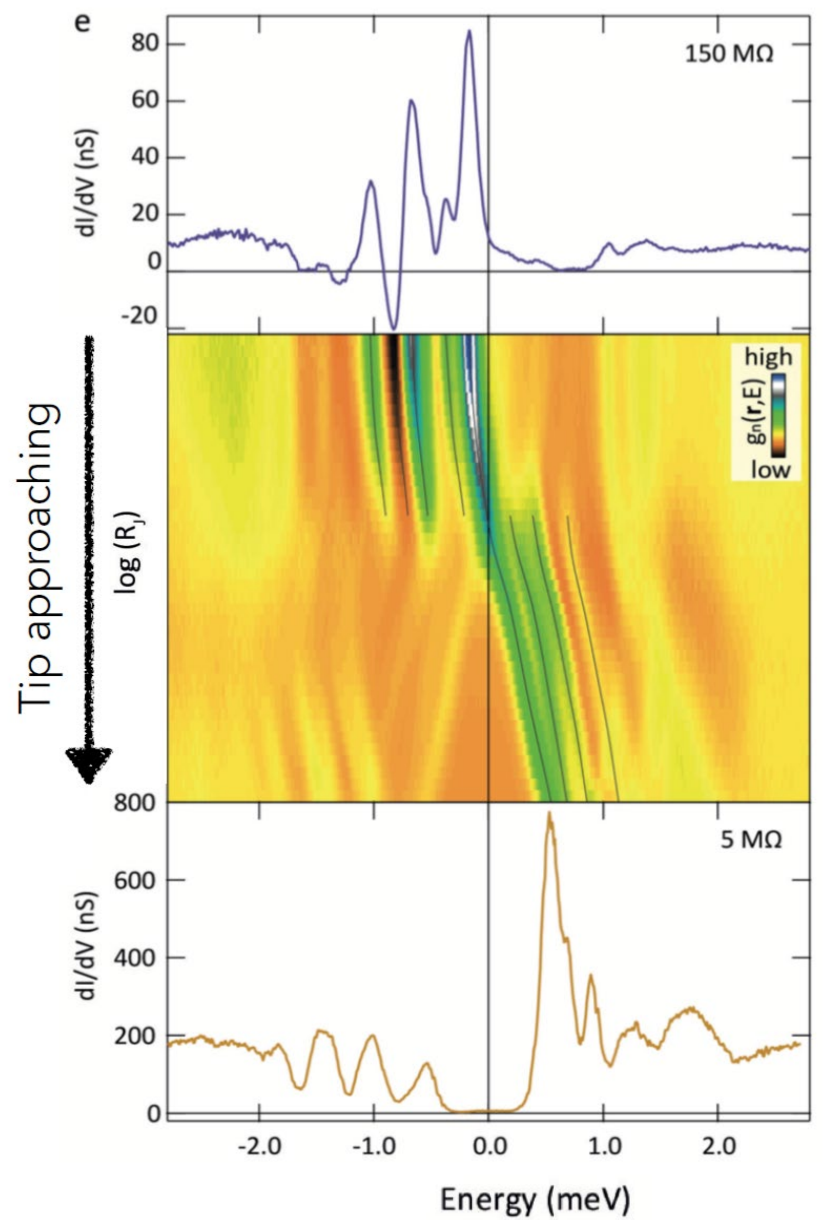
Compelling experimental evidence that Fe(Te,Se) is a **gapped** superconductor

We will consider a **minimal *s*-wave** model

Experimental observations

T=0.3 K





- **Multiple** in-gap states
- **Tunable** energy

Low density of carriers ⟹ Poor screening

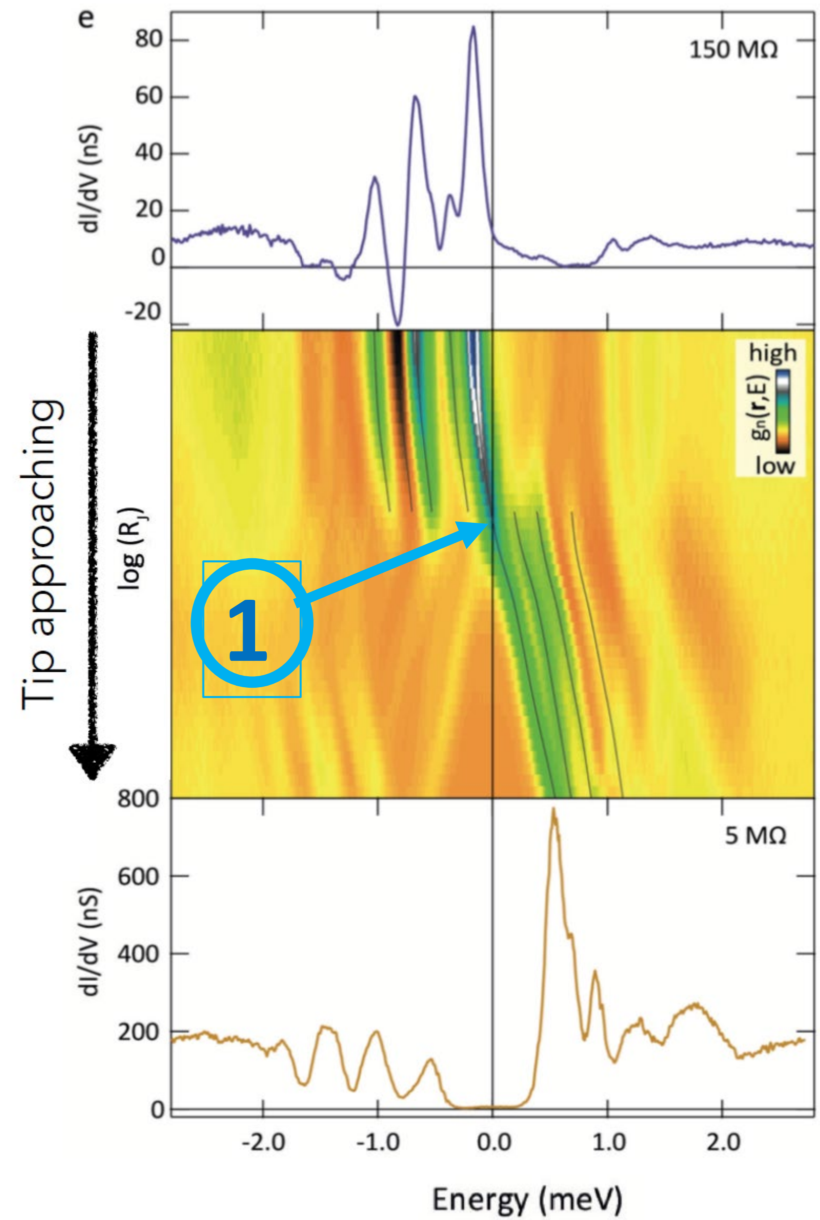
Assumption: Tip acts as a local gate electrode

Experimental observations

Two key features:

1) Concurrent switch of in-gap states from hole-like to electron-like

Independent classical YSR channels



Experimental observations

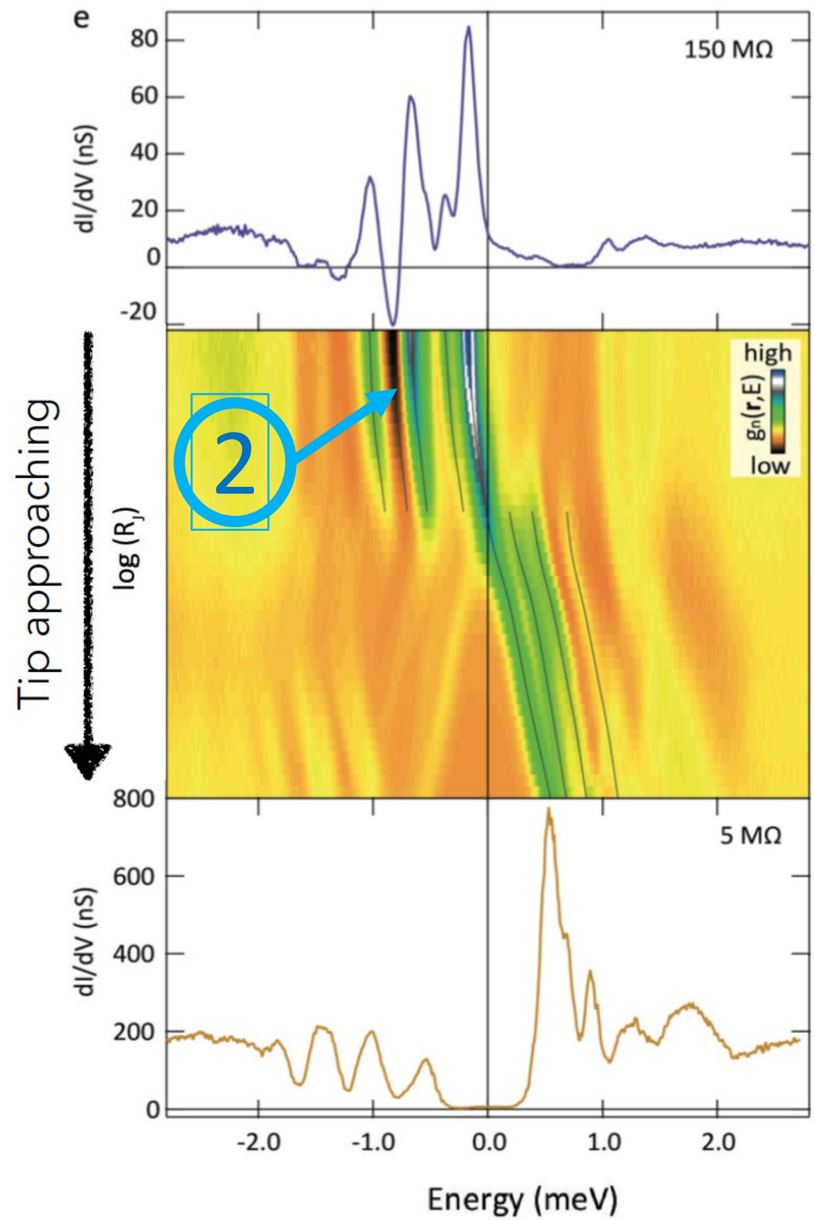
Two key features:

1) Concurrent switch of in-gap states from hole-like to electron-like

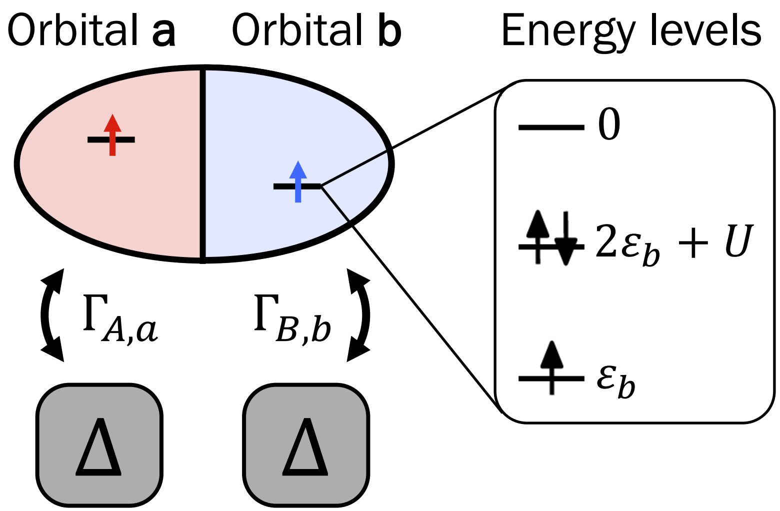
Independent classical YSR channels

2) Appearance of negative differential conductance (NDC)

Multiple impurity states and Coulomb interaction



Multi-channel Anderson impurity model



$$\Gamma_{i,\alpha} = \pi t_{i,\alpha}^2$$

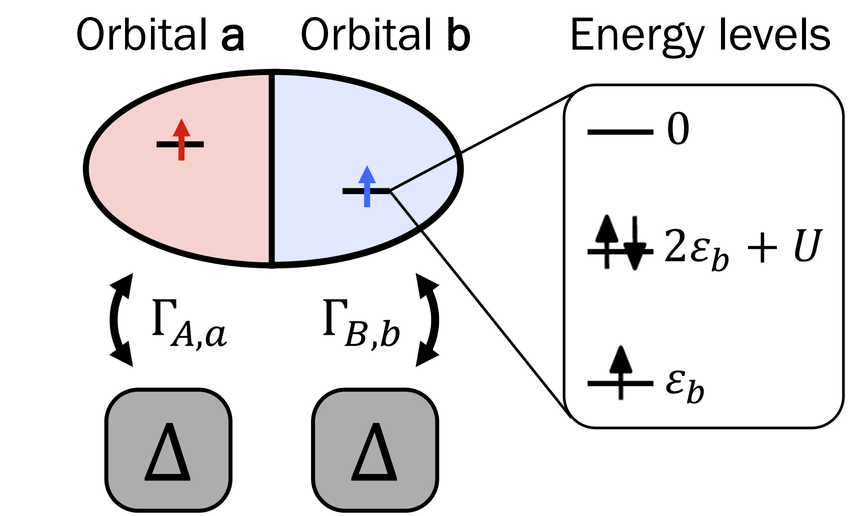
$$H = H_{SC} + H_T + H_{imp}$$

$$H_{SC} = \sum_{i=A,B} \left(\Delta c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger + \Delta^* c_{i,\downarrow} c_{i,\uparrow}\right)$$

$$H_T = \sum_{i,\alpha,\sigma} \left(t_{i,\alpha} c_{i,\sigma}^\dagger d_{\alpha,\sigma} + t_{i,\alpha}^* d_{i,\sigma}^\dagger c_{\alpha,\sigma}\right)$$

$$H_{imp} = \sum_{\alpha,\sigma} \varepsilon_\alpha d_{\alpha,\sigma}^\dagger d_{\alpha,\sigma} + \sum_{\alpha} \left(U_\alpha d_{\alpha,\uparrow}^\dagger d_{\alpha,\uparrow} d_{\alpha,\downarrow}^\dagger d_{\alpha,\downarrow}\right)$$

Multi-channel
Anderson impurity model



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$$H_{SC} = \sum_{i=A,B} \left(\Delta c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger + \Delta^* c_{i,\downarrow} c_{i,\uparrow} \right)$$

$$H_T = \sum_{i,\alpha,\sigma} \left(t_{i,\alpha} c_{i,\sigma}^\dagger d_{\alpha,\sigma} + t_{i,\alpha}^* d_{i,\sigma}^\dagger c_{\alpha,\sigma} \right)$$

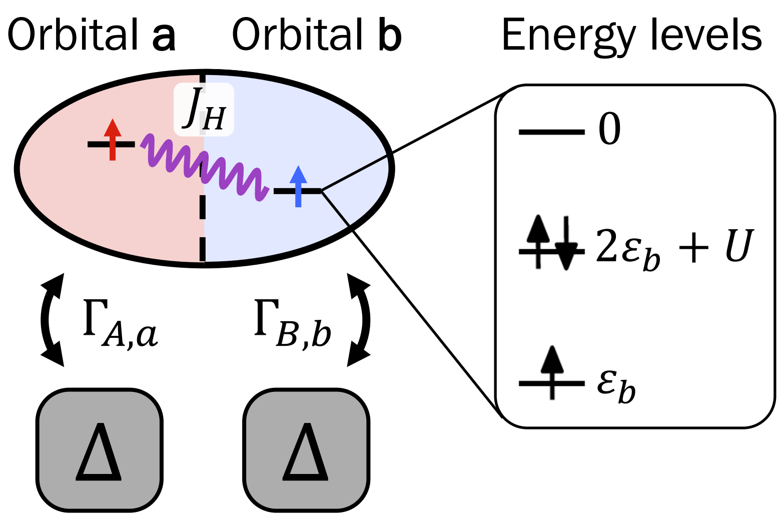
$$H_{imp} = \sum_{\alpha,\sigma} \varepsilon_\alpha d_{\alpha,\sigma}^\dagger d_{\alpha,\sigma} + \sum_\alpha \left(U_\alpha d_{\alpha,\uparrow}^\dagger d_{\alpha,\uparrow} d_{\alpha,\downarrow}^\dagger d_{\alpha,\downarrow} \right)$$

$$\bar{\varepsilon} = \frac{\varepsilon_a + \varepsilon_b}{2}$$

‘crystal field’ splitting $\delta\varepsilon = \varepsilon_a - \varepsilon_b = \mathrm{C}$

$\bar{\varepsilon}$ varies linearly with tip-sample distance

Multi-channel
Anderson impurity model



$\Gamma_{i,\alpha} = \pi t_{i,\alpha}^2$

$$H = H_{SC} + H_T + H_{imp}$$

$$H_{SC} = \sum_{i=A,B} \left(\Delta c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger + \Delta^* c_{i,\downarrow} c_{i,\uparrow} \right)$$

$$H_T = \sum_{i,\alpha,\sigma} \left(t_{i,\alpha} c_{i,\sigma}^\dagger d_{\alpha,\sigma} + t_{i,\alpha}^* d_{i,\sigma}^\dagger c_{\alpha,\sigma} \right)$$

$$H_{imp} = \sum_{\alpha,\sigma} \varepsilon_\alpha d_{\alpha,\sigma}^\dagger d_{\alpha,\sigma} + \sum_\alpha \left(U_\alpha d_{\alpha,\uparrow}^\dagger d_{\alpha,\uparrow} d_{\alpha,\downarrow}^\dagger d_{\alpha,\downarrow} - J_H \hat{\boldsymbol{S}}_{\boldsymbol{a}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{b}} \right)$$

$$\bar{\varepsilon} = \frac{\varepsilon_a + \varepsilon_b}{2}$$

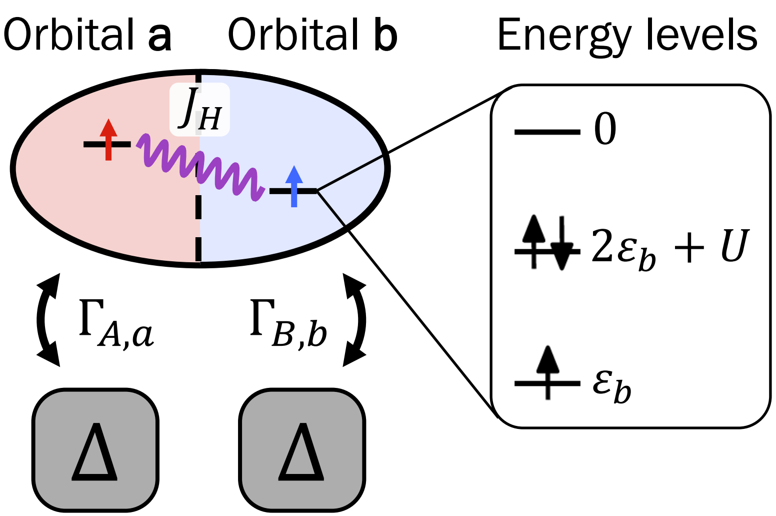
Hund's coupling
$J_H > 0$

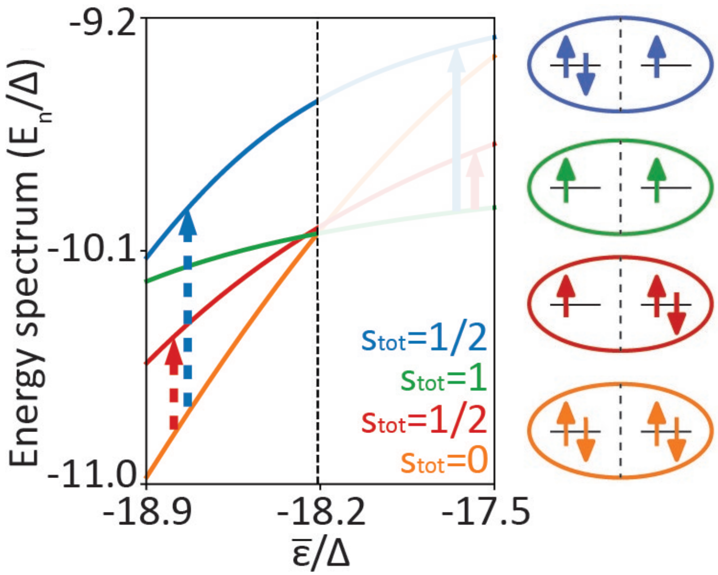
$U \sim |\bar{\varepsilon}| > |J_H| > |\delta\varepsilon| \gtrsim \sqrt{\Gamma_{i,\alpha}} > \Delta$

'crystal field' splitting $\delta\varepsilon = \varepsilon_a - \varepsilon_b = \mathrm{C}$

$\bar{\varepsilon}$ varies linearly with tip-sample distance

Multi-channel Anderson impurity model: many-body spectrum





$\Gamma_{i,\alpha} = \pi t_{i,\alpha}^2$

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'crystal field' splitting $\delta\varepsilon = \varepsilon_a - \varepsilon_b = \mathrm{C}$

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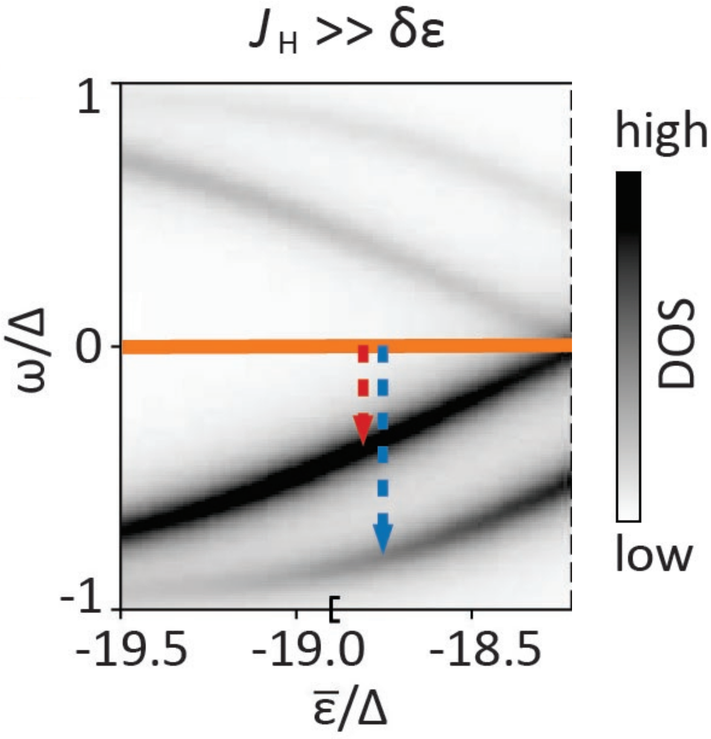
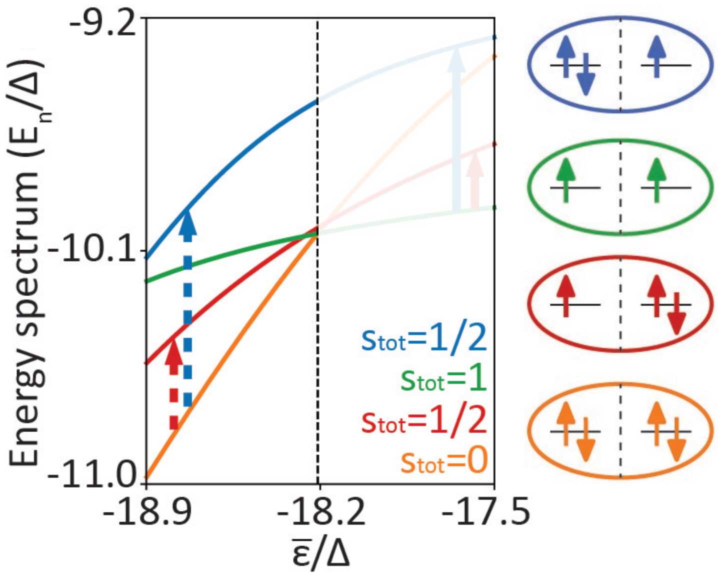
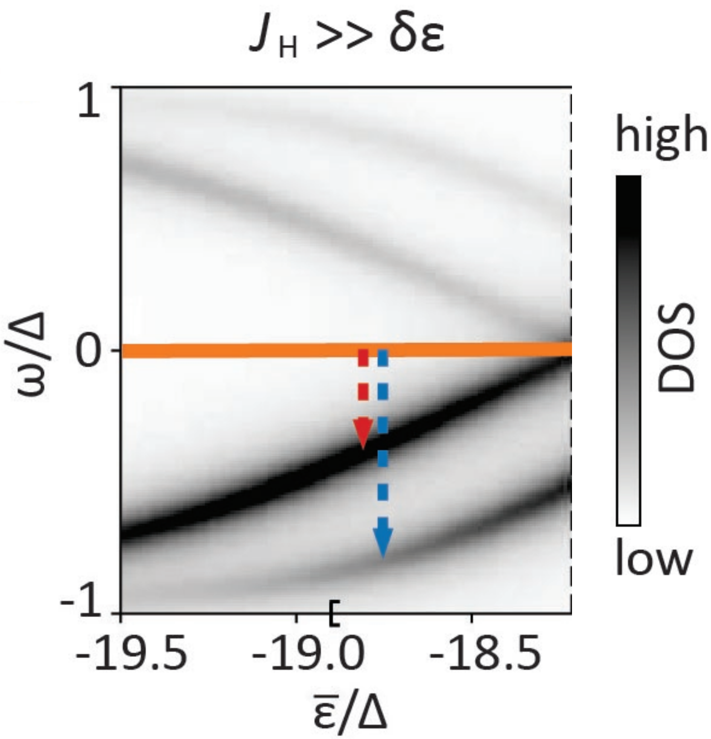
Multi-channel Anderson impurity model: many-body spectrum

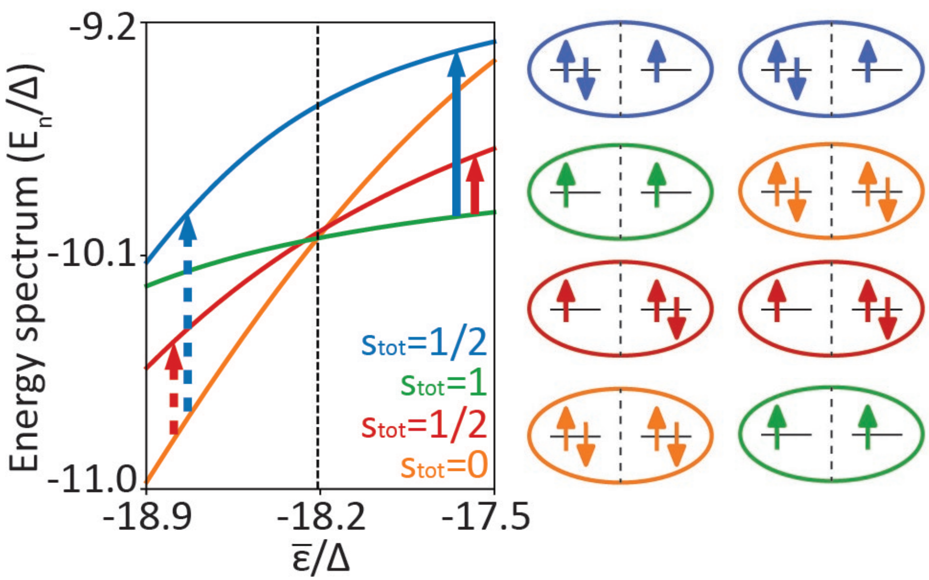




M. Uldemolins et al., Nature Comm 15, 8526 (2024)

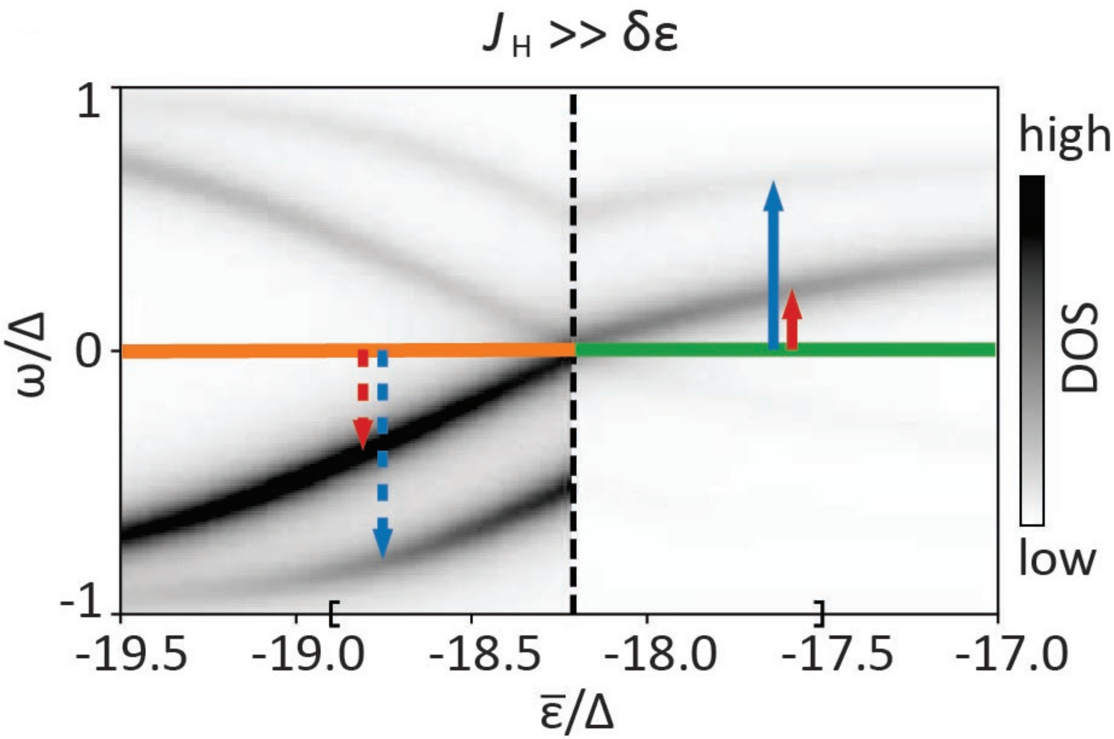
Multi-channel
Quantum phase transition

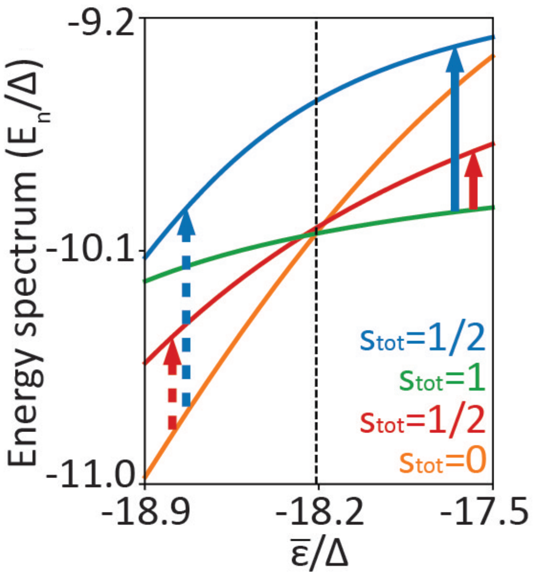




- Multi-channel quantum phase transition: large change in occupation
- Orbital energy cost compensated by gain of Hund's energy

Multi-channel
Quantum phase transition





- Calculated LDOS captures STM experiment

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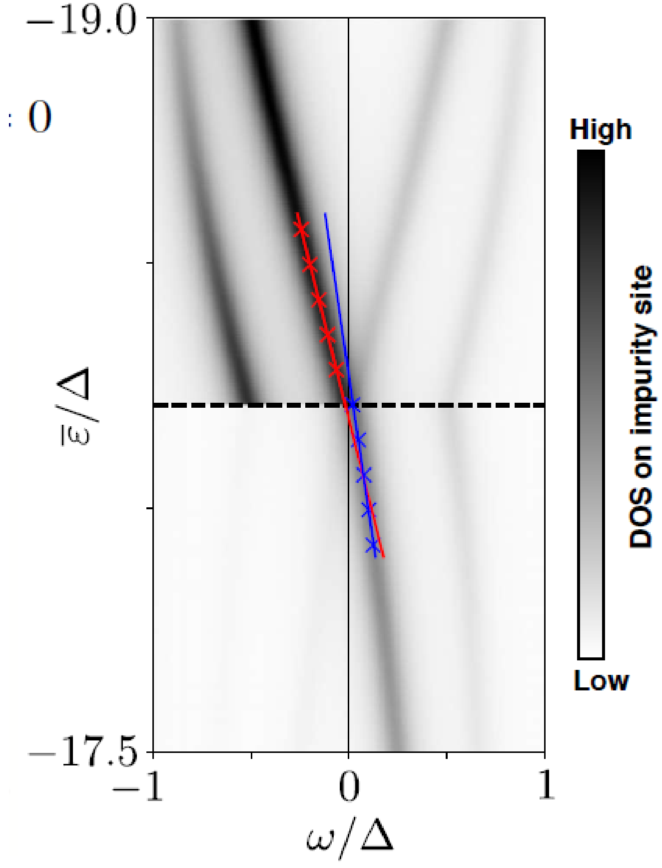
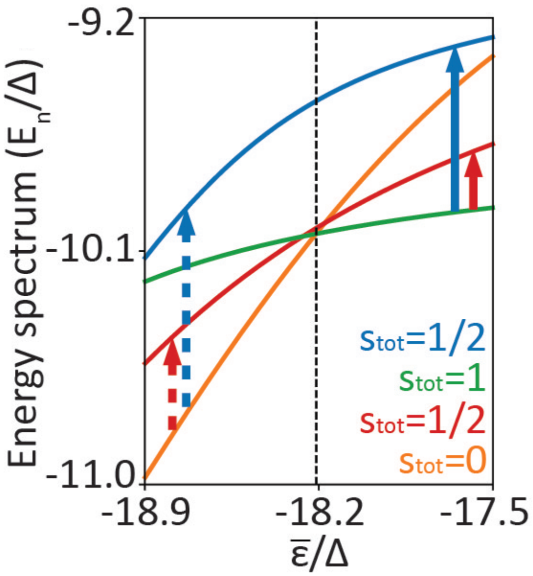
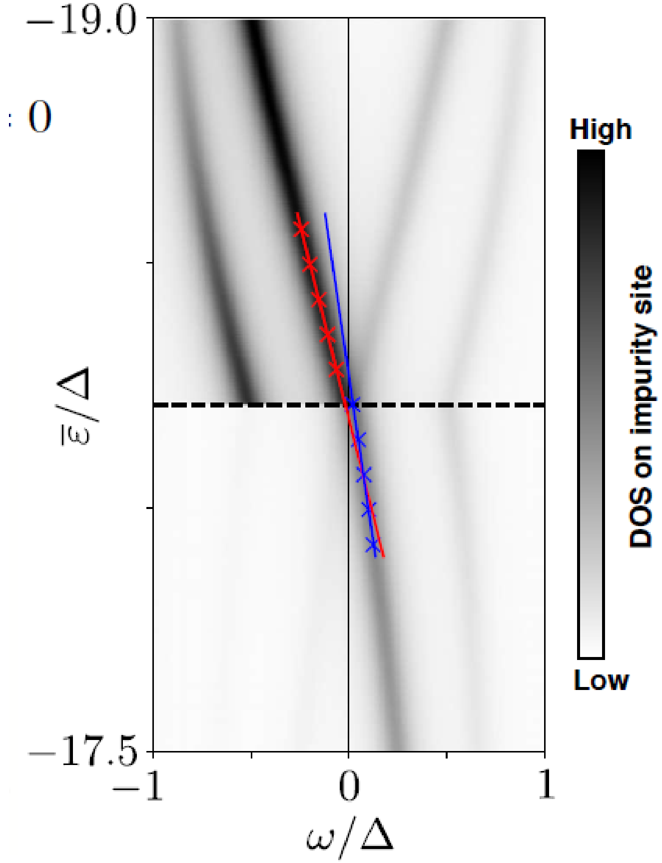
Slope changes upon crossing E=0

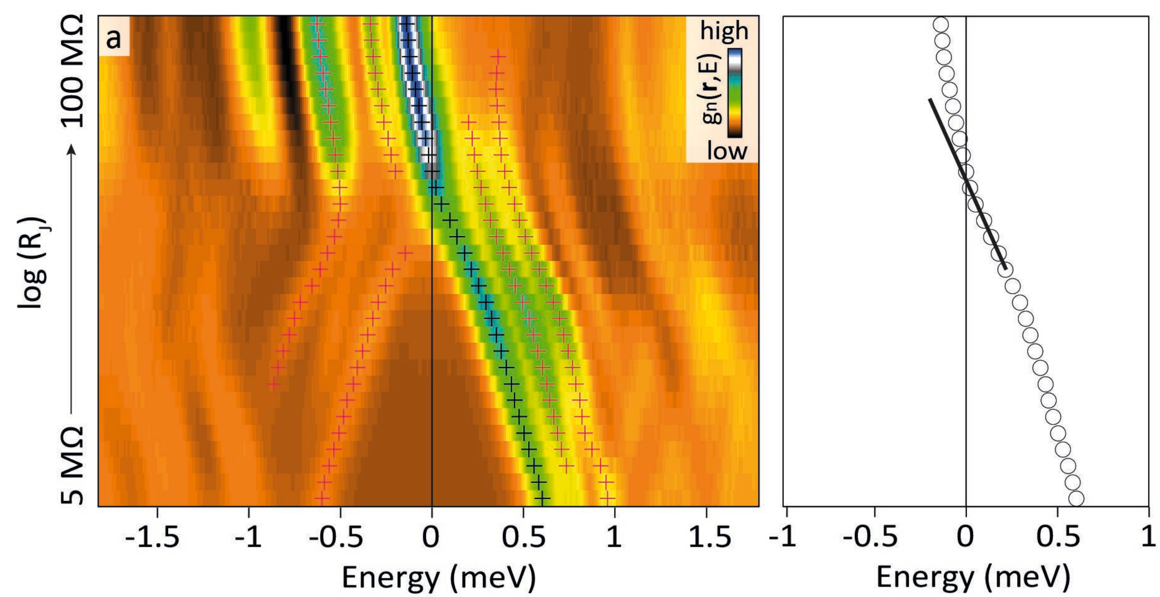




- Discontinuous slope at E = 0

Slope changes upon crossing E=0

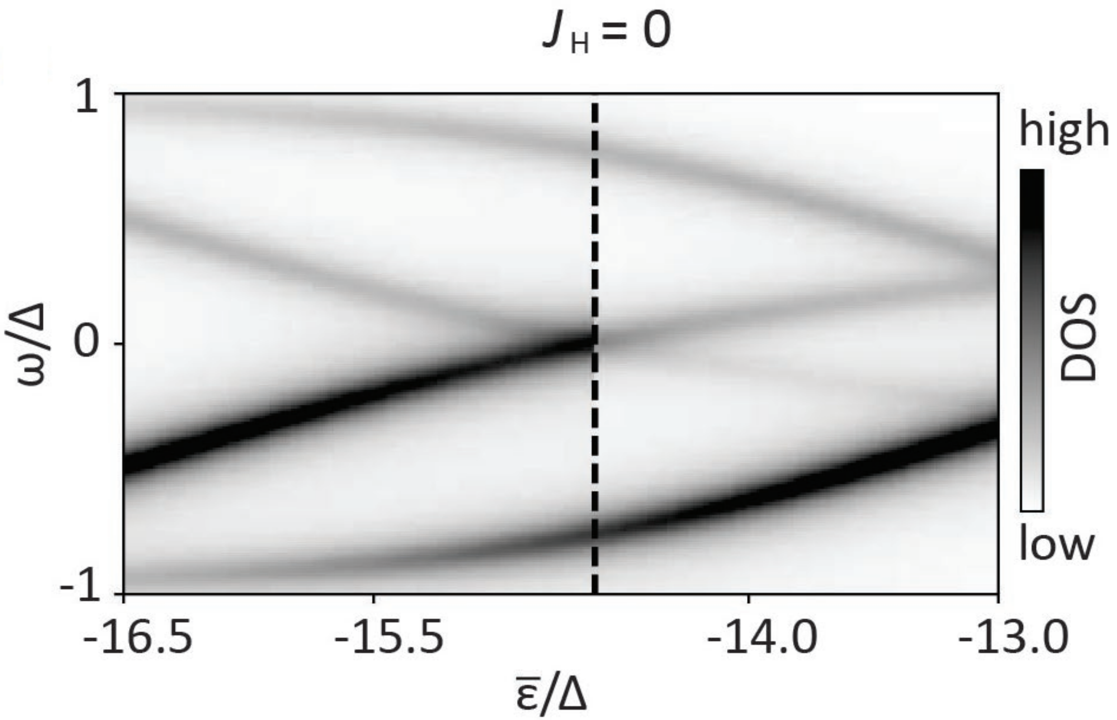




- Discontinuous slope at E = 0

M. Uldemolins et al., Nature Comm 15, 8526 (2024)

Switching off the Hund coupling



Comparison to $J_H = 0$:
orbitals decoupled,
similar to independent
YSR or Kondo channels

- $J_H = 0$ does **not** match the experiment

M. Uldemolins et al., Nature Comm 15, 8526 (2024)

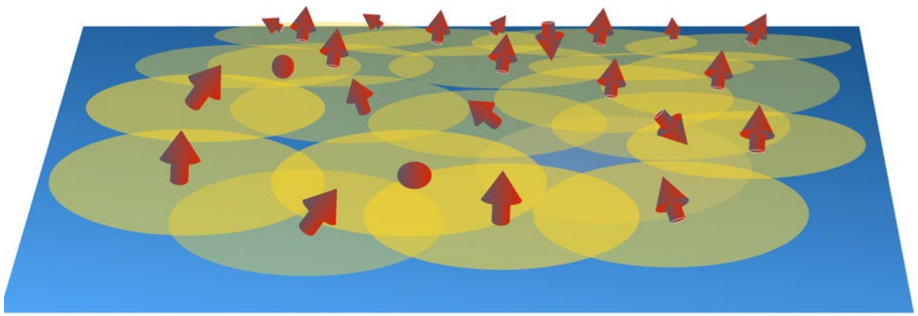
Multi-channel quantum phase transition (MCQPT)

Independent YSR channels not always suitable

- High spin impurities (Hund's coupling)
- Large change in ground state occupation at MCQPT
- Discontinuity of both the slope and intensities at the transition

Questions: dynamical control ?

Engineering amorphous superconductivity



Assume deep Shiba band and project onto it

→ Maps on a 2D effective chiral topological superconductor

$$H_{mn} = \begin{pmatrix} h_{mn} & \Delta_{mn} \\ (\Delta_{mn})^\dagger & -h^*_{mn} \end{pmatrix}$$

$$h_{mn}, \Delta_{mn} \sim \frac{e^{-r_{mn}/\xi}}{\sqrt{r_{mn}}}$$

However with **long range hopping and pairing**

→ Consequence of long-range spatial extent of the YSR states

See e.g. ``Amorphous topological superconductivity in a Shiba glass'',
K. Pöyhönen et al., Nat. Comm. 9, 2103 (2018)