From the single magnetic impurity dynamics in a Superconductor to the YSR qubit

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University Paris Saclay

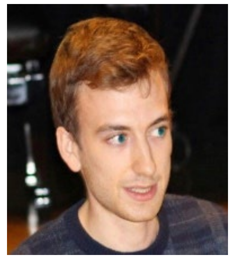
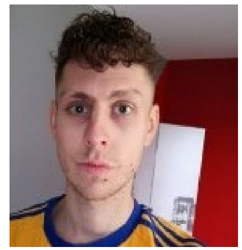
QSPICE Workshop Quantum Functionalities of Nanomagnets, Ingelheim, 18-06-25

Main Collaborators

Part 1

LPS Theory CNRS & University Paris Saclay

- **Mateo Uldemolins**
- **Vivien Perrin**
- Andrej Mesaros


IMN Nantes

- Laurent Cario

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




Genda Gu

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Part 2

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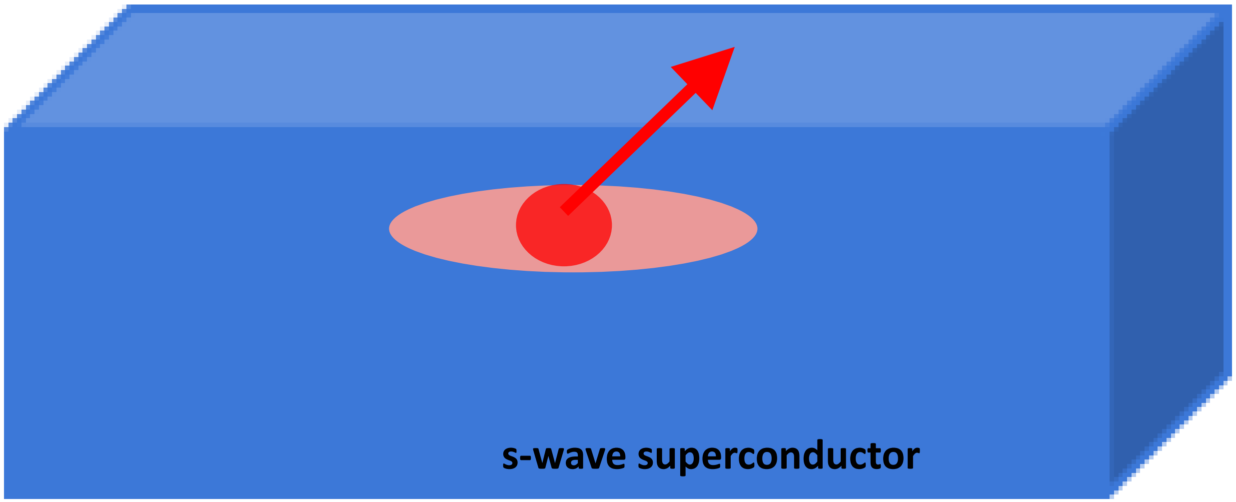
So Takei, CUNY

Timo Hyart, Aalto

Why studying magnetic impurities in a superconductor ?

An old solved problem ?

Atom with a magnetic moment:
Fe, Co, Mn



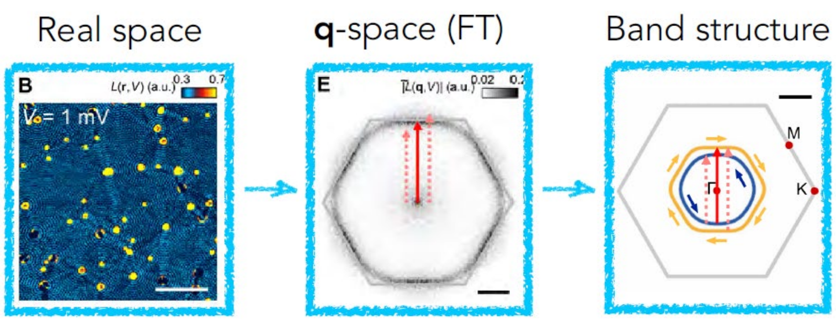
Magnetic adatom: pair-breaking defect

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).

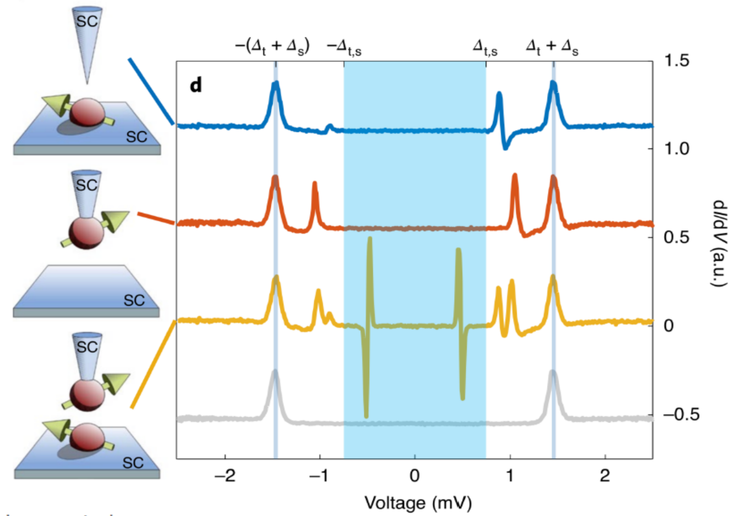
Motivation 1: Local defects as probing tools

Quasiparticle Interference (QPI)



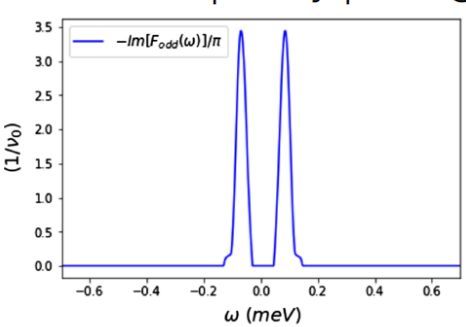
Yim et al. Sci. Adv. 7 eabd7361 (2021)

YSR-state functionalized tips



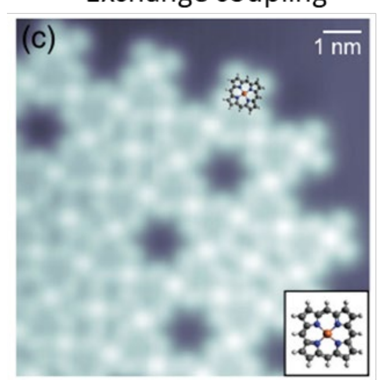
Huang et al.
Nat. Phys. 16, 1227-1231 (2020)

Odd-frequency pairing



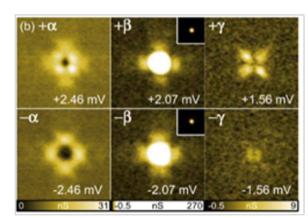
Perrin et al.
PRL 125, 117003 (2020)

Exchange coupling



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

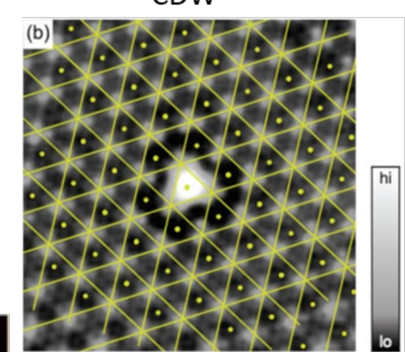
Orbitals



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

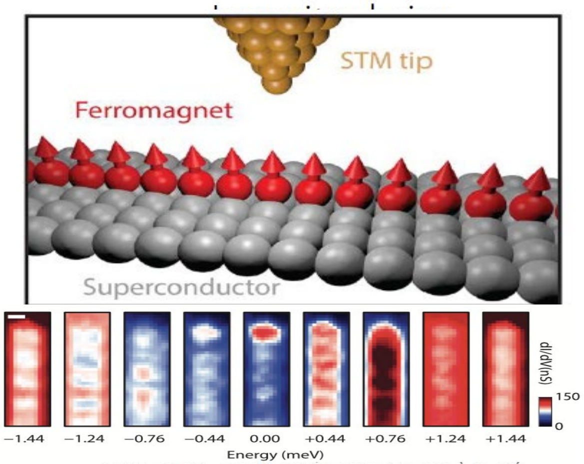
D.J.Choi et al.
Nat.Comm. 8 15175(2017)

CDW



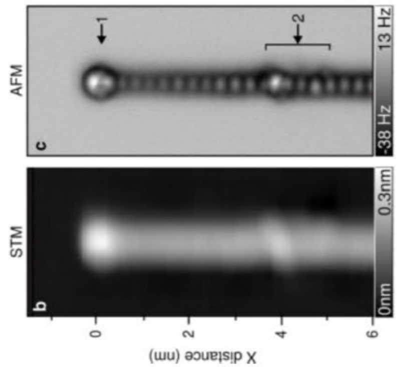
E.Liebhaber et al.
Nano. Lett. 20, 339(2020)

Motivation 2: Engineering exotic states



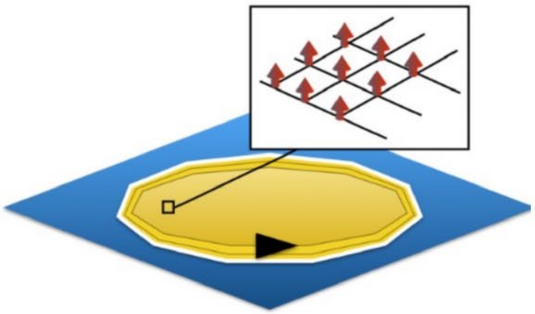
S. Nadj-Perge et al., Science **346,** 6209 (2014)

Majorana states



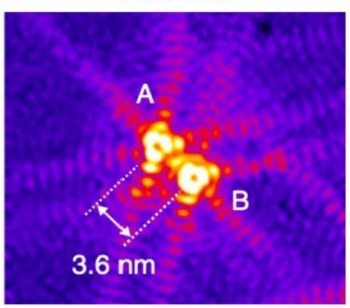
Pawlak et al. npj Q. Info 2, 16035 (2016)

Impurity lattices for topological SC

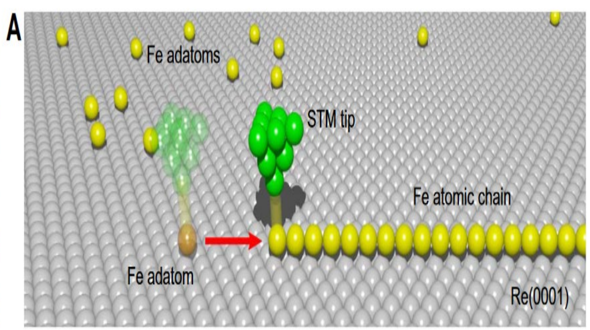


Rontynen, Ojanen. PRB 93, 094521 (2016)

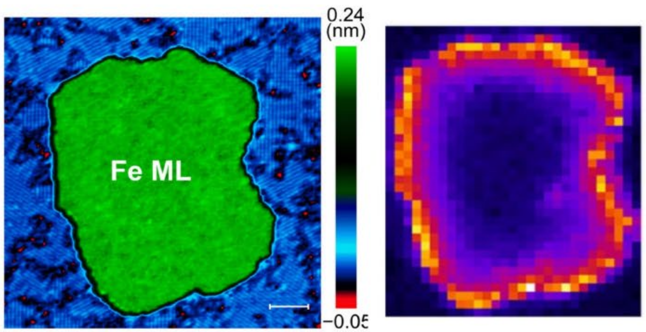
Dimers



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

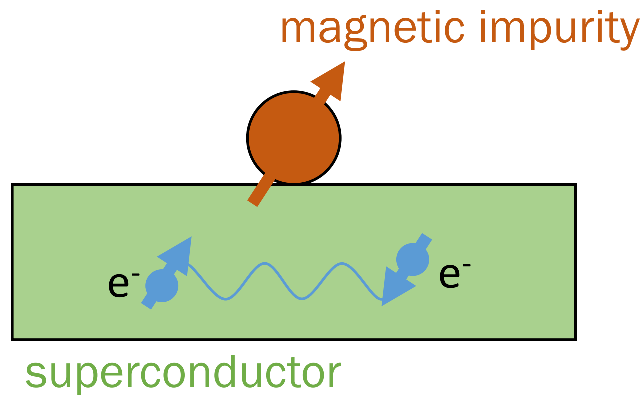


Kim et al. Sci. Adv., **2** eaar5251 (2018)



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

Questions ?



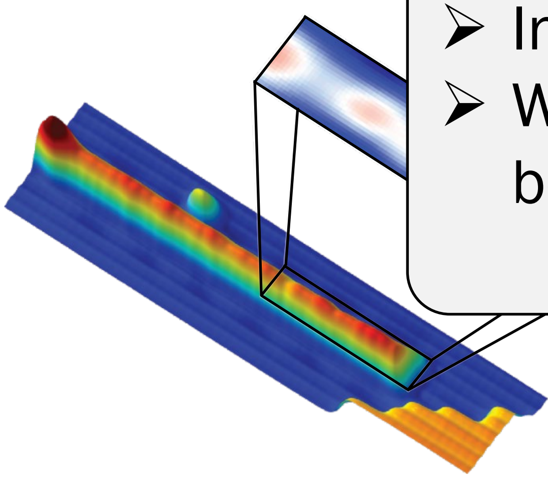
- As a probe of bulk properties
- As a building block

Chains & ladd

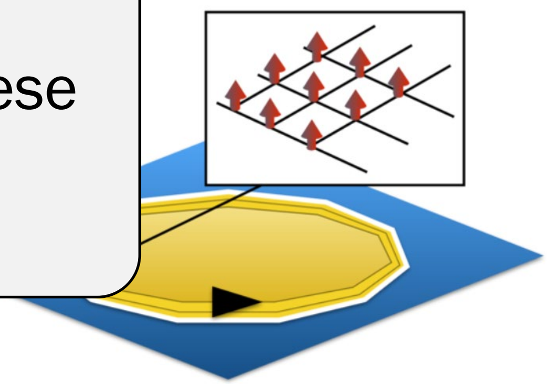
Majorana end s

lattices:

superconductivity



- Relaxation (lifetime)
- Interactions
- What to do with these bound states ?



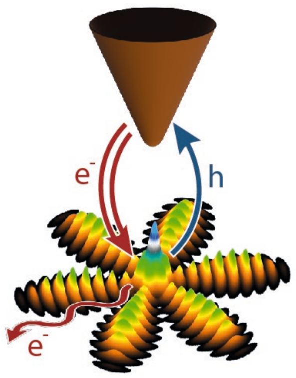
PRB **93**, 094521 (2016)

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

Today's menu

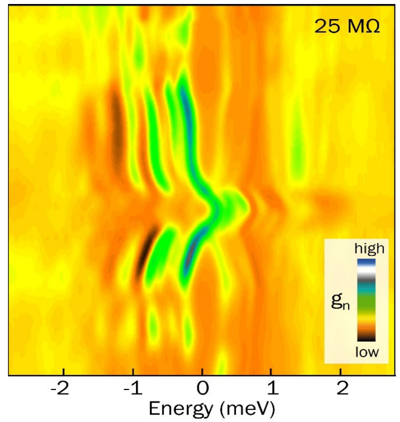
1. Lifetime of sub-gap states

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

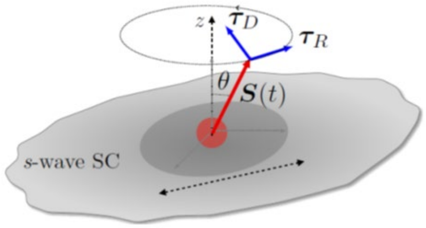


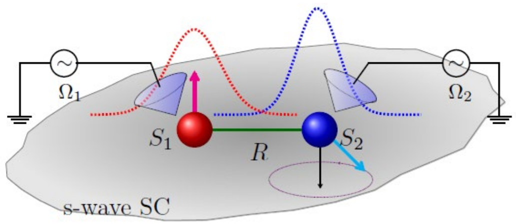
2. Multi-channel quantum phase transition

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



3. Toward a YSR qubit





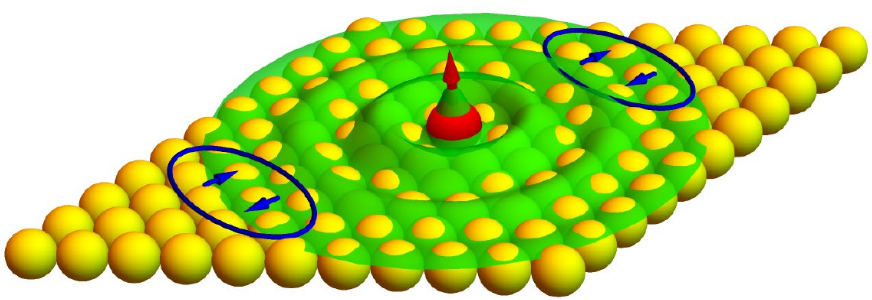
A. Mischra et al. , PRB **103**, L121401 (2021)); PRX Quantum **2,** 040347 (2021)

A magnetic impurity in a superconductor

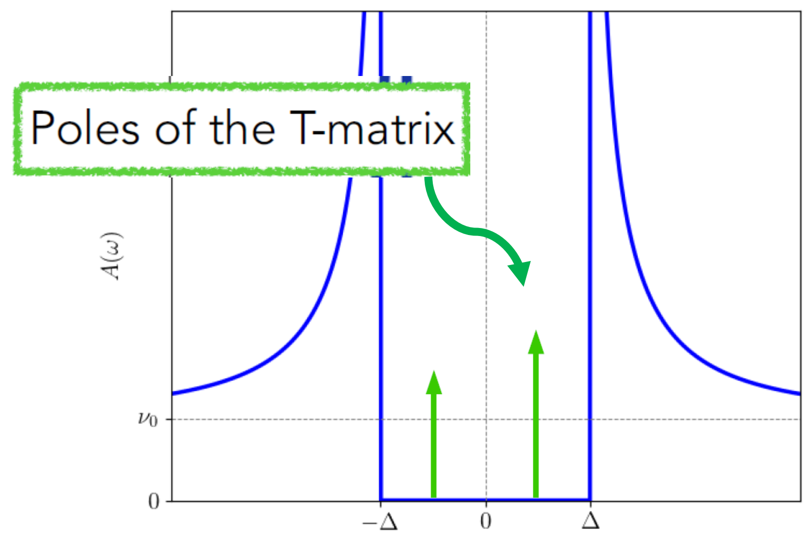
$$H = \sum_{\mathbf{k}\sigma} \xi_k c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \Delta \sum_{\mathbf{k}} \left(c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \right) - J \left(c^\dagger_{0\uparrow} c_{0\uparrow} - c^\dagger_{0\downarrow}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

Assumptions about the impurity

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



Assumes Δ constant
(homogeneous))

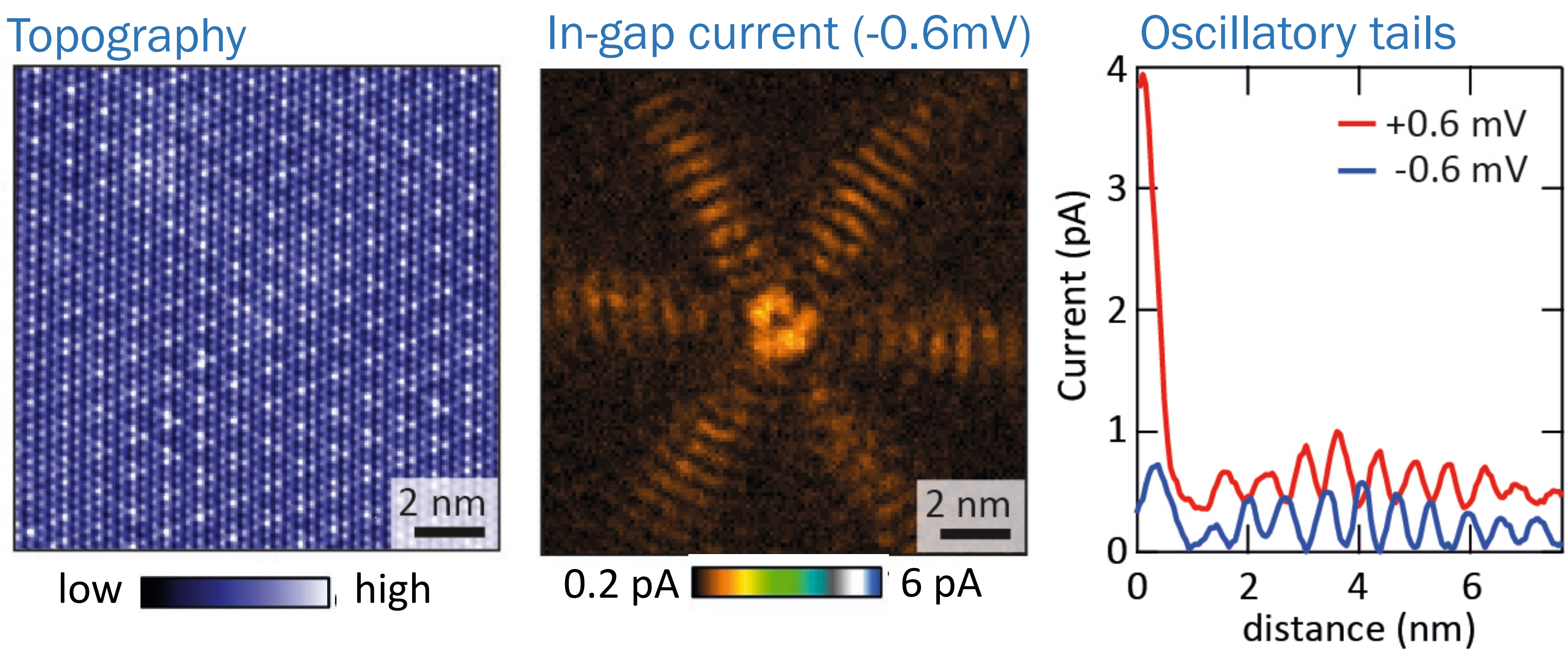


YSR (K=0)

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

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

Extended YSR in NbSe2



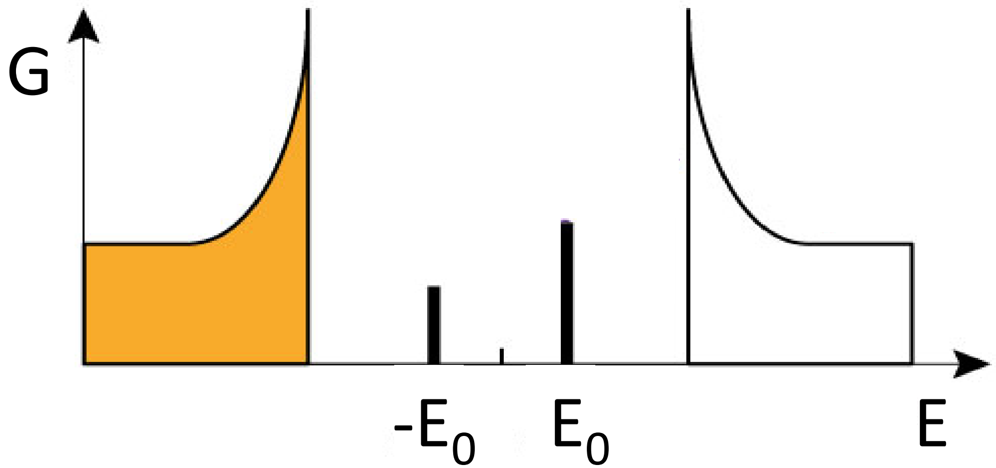
U. Thupakula et al., Phys. Rev. Lett. **128**, 247001 (2022)

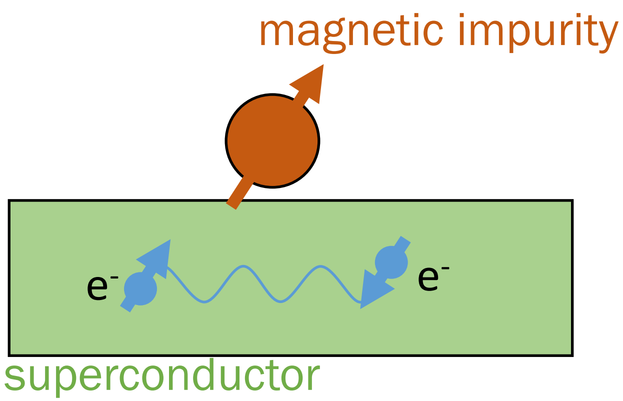
see also Ménard et al., *Nat. Phys.* **11**, 1013 (2015)

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 ?





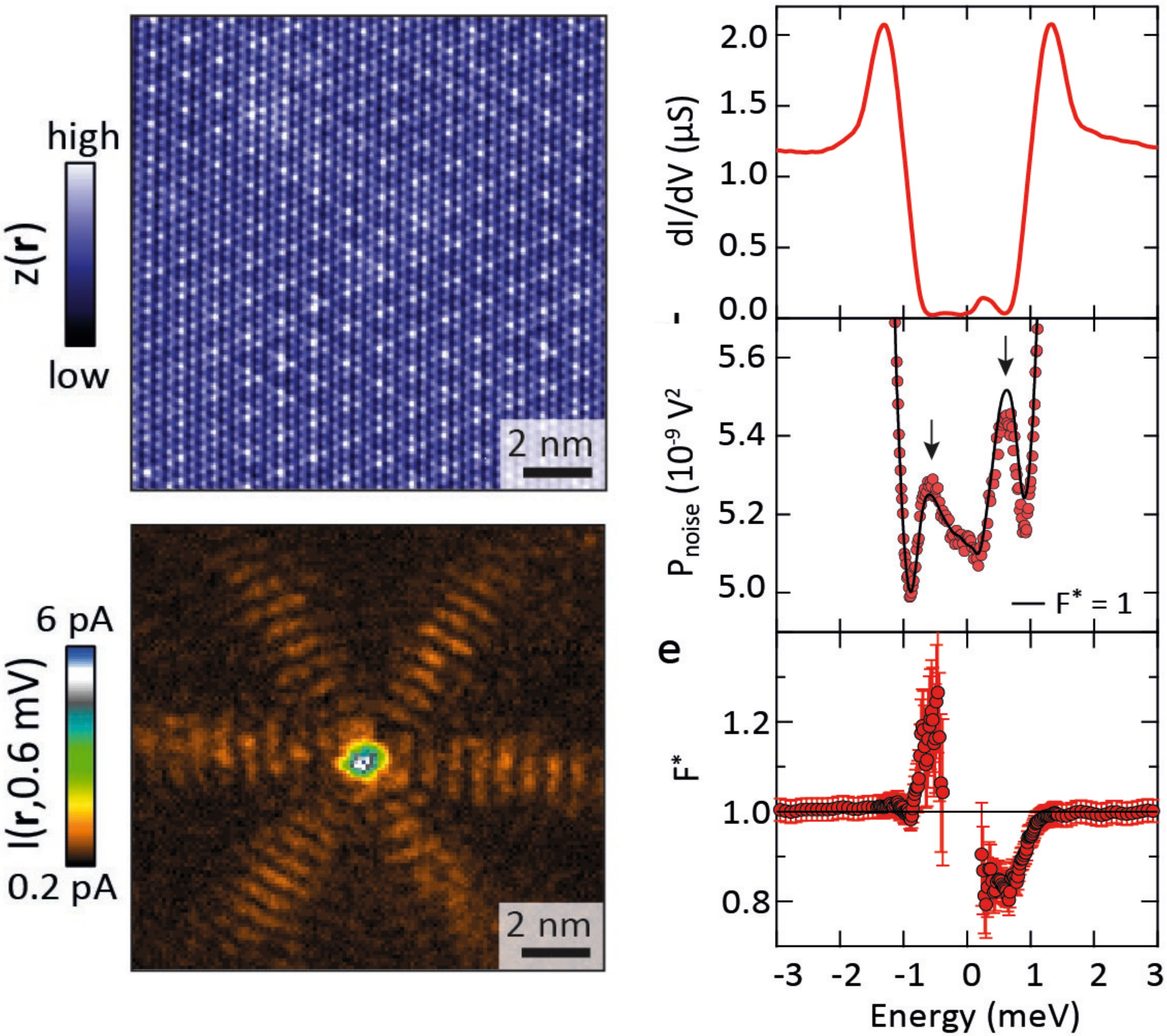
Science **275**, 1767 (1997)
PRL **100**, 2268 (2008)
Nat. Phys. **11**, 1013 (2015)
PRL **115**, 087001 (2015)
...

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 ?

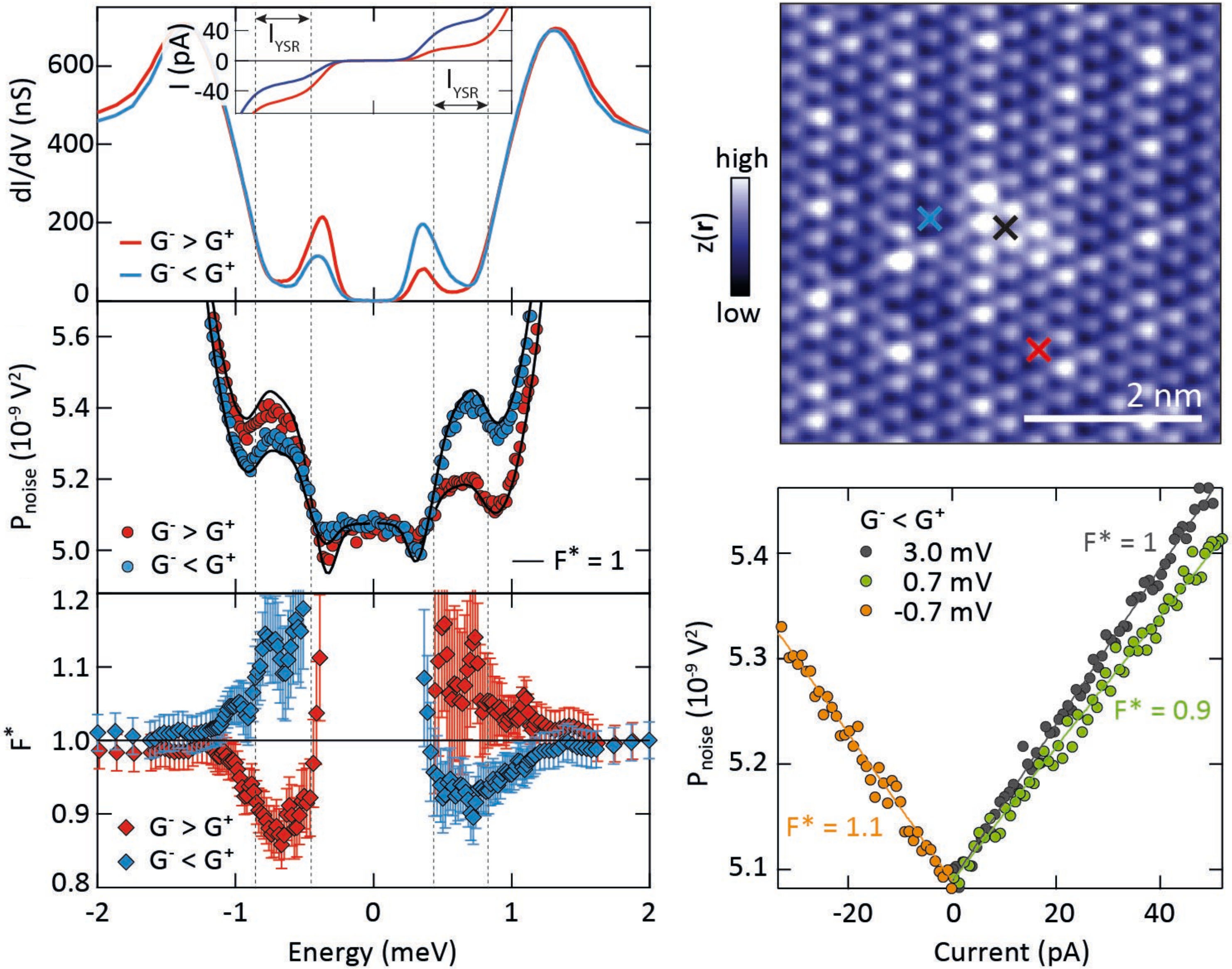
Noise tomography of YSR states in 2H-$NbSe_2$



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

U. Thupakula et al., PRL (2022)

Noise tomography of YSR states in $2H\text{-}NbSe_2$



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

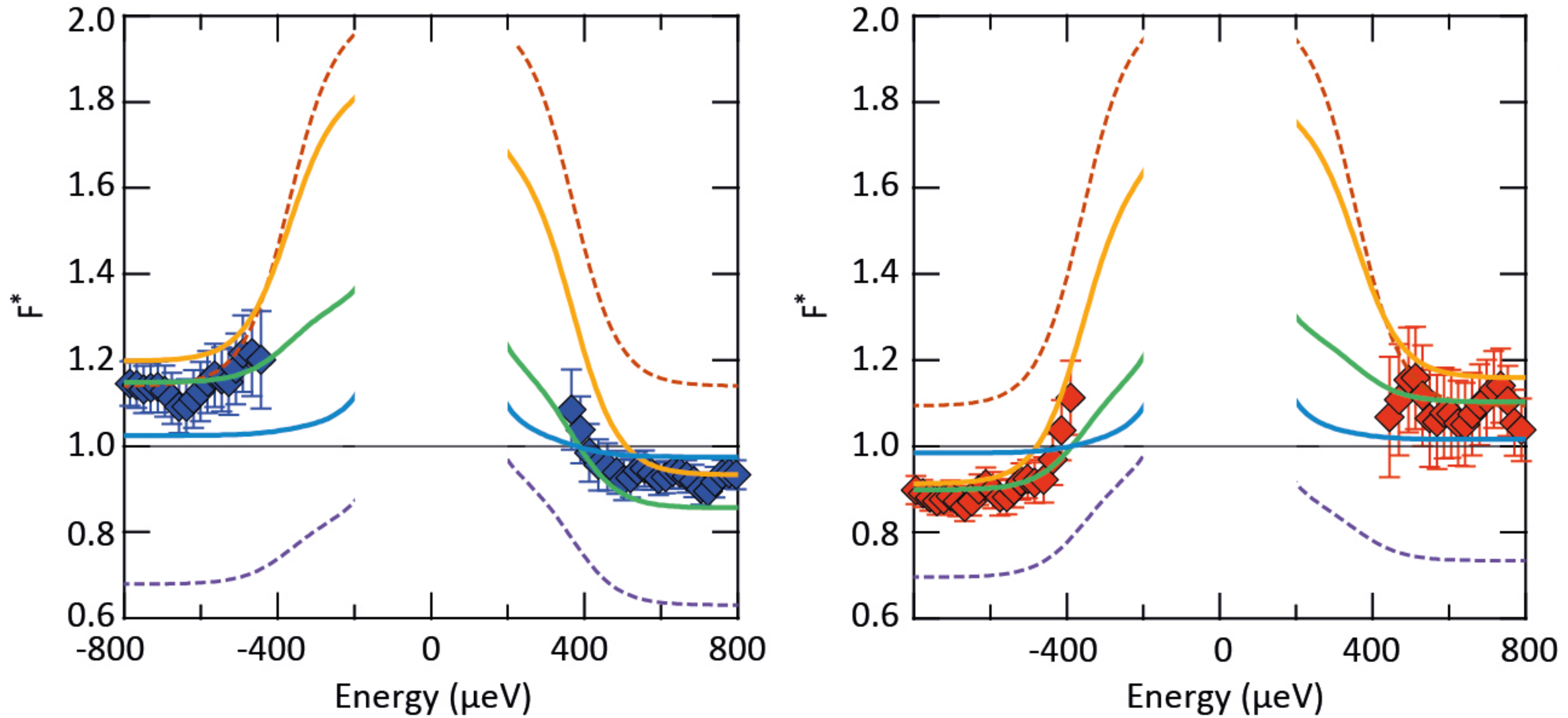
using model from *PRL* **115**, 087001 (2015)

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

intrinsic life-time

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

$3.5k_BT = 200\ \mu eV$

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

Impurity models

Complexity →

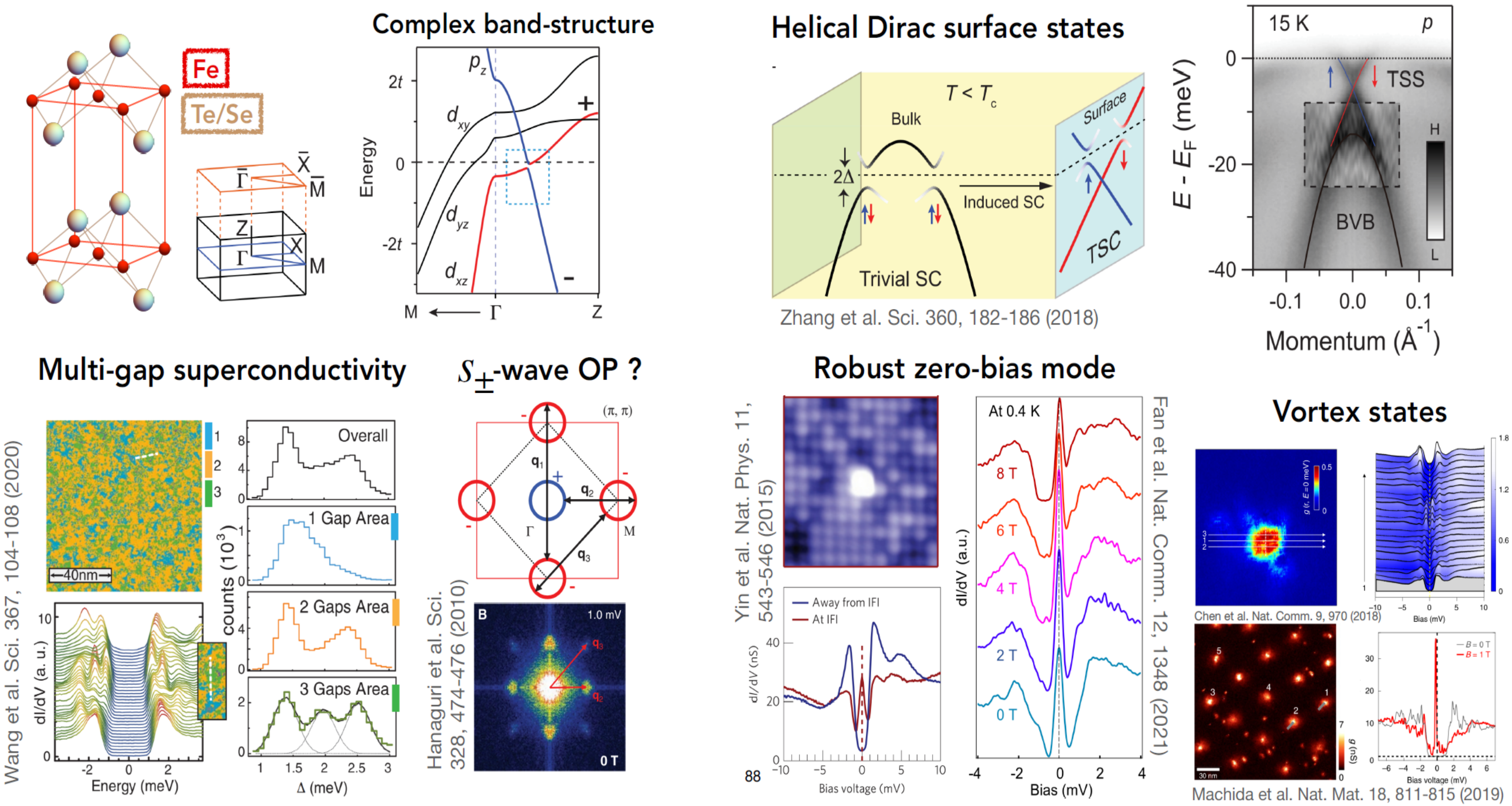
Classical spin

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

- 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

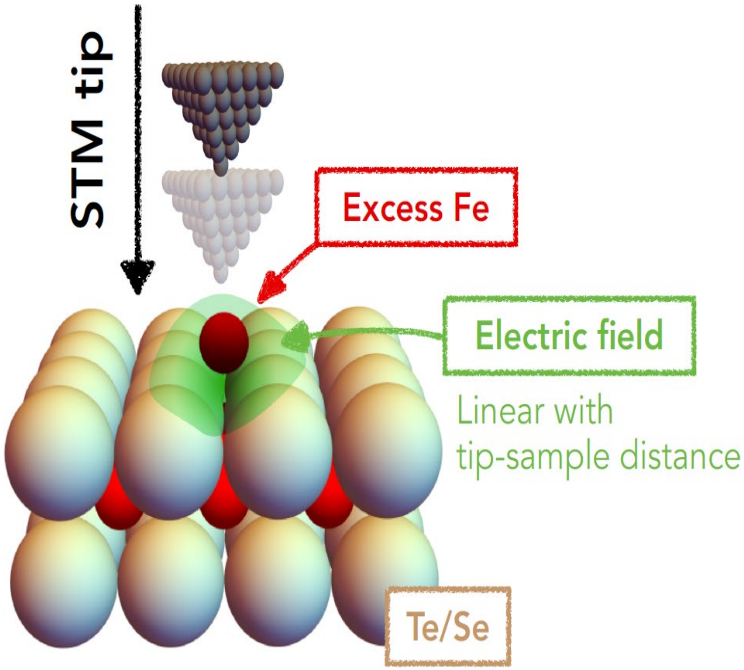


Compelling experimental evidence that Fe(Te,Se) is a **gapped** superconductor

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

Experimental observations

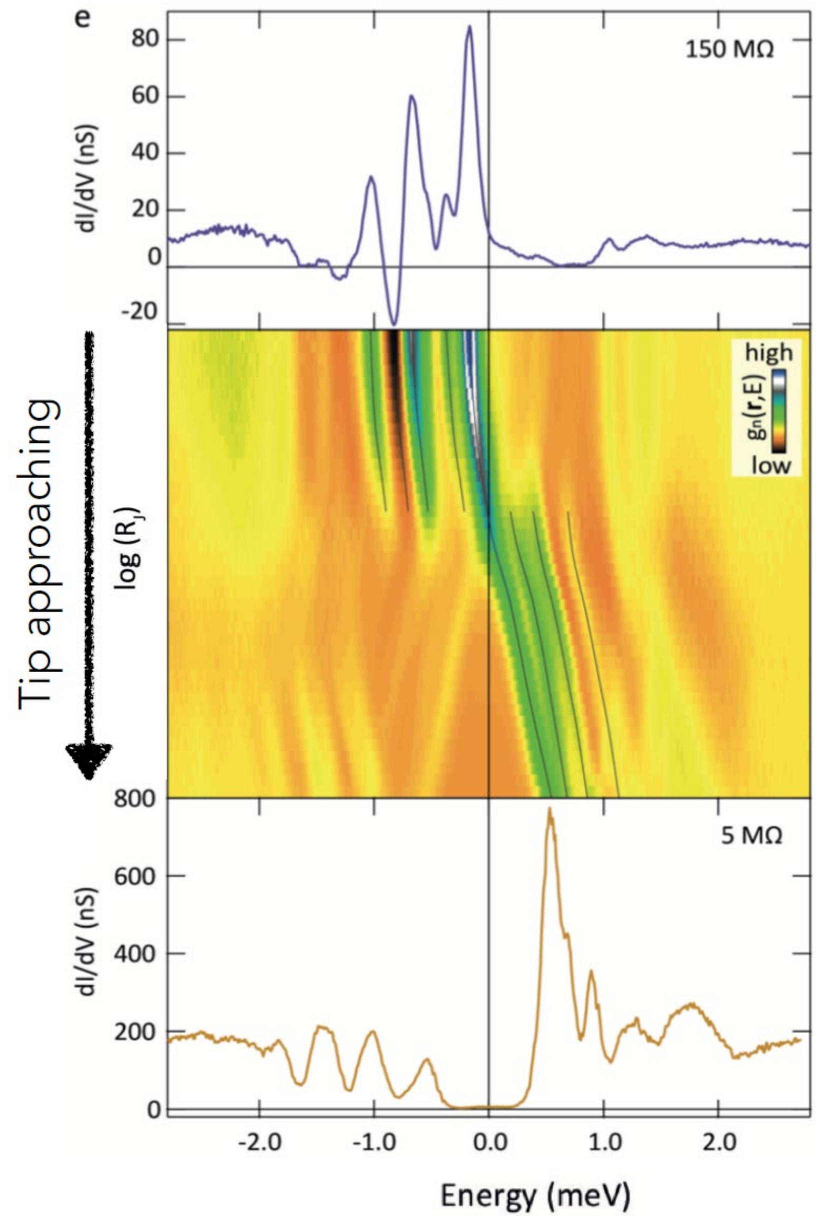
T=0.3 K



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

Low density of carriers ⇒ Poor screening

Assumption: Tip acts as a local gate electrode

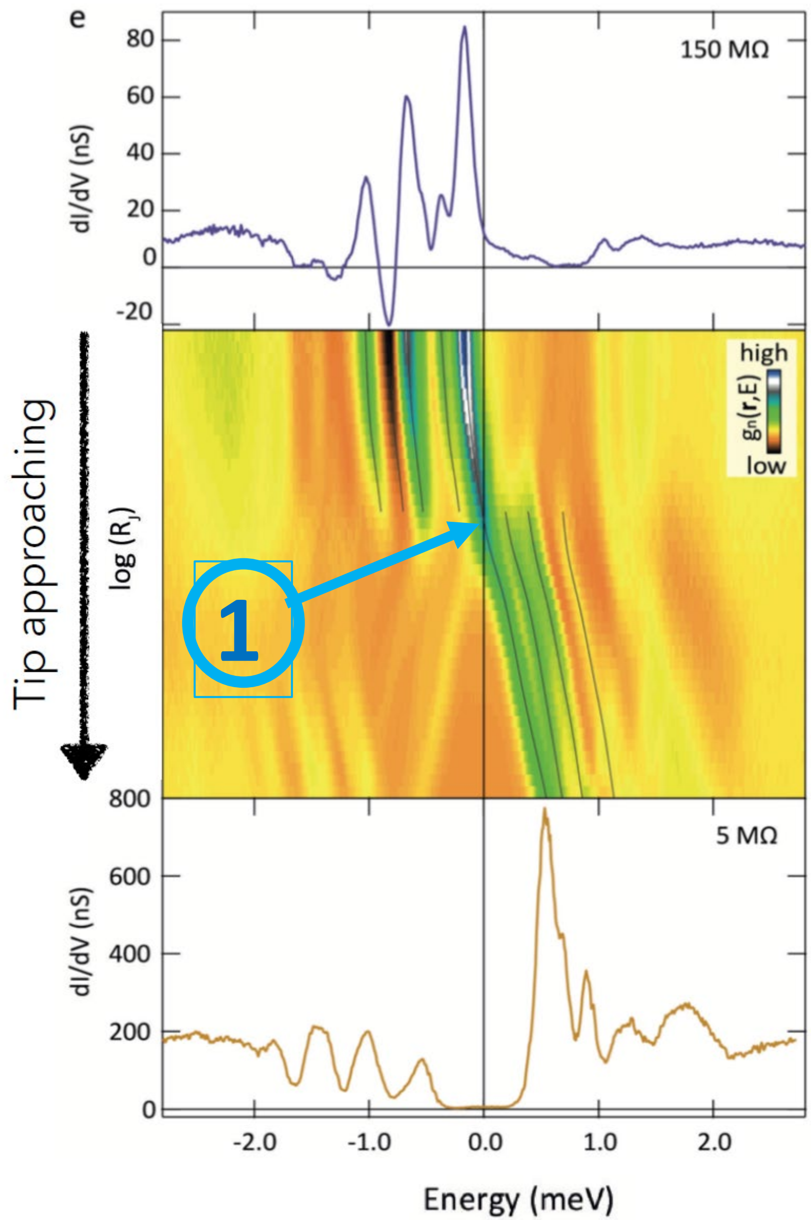


Experimental observations

Two key features:

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

Independent classical YSR channels



Experimental observations

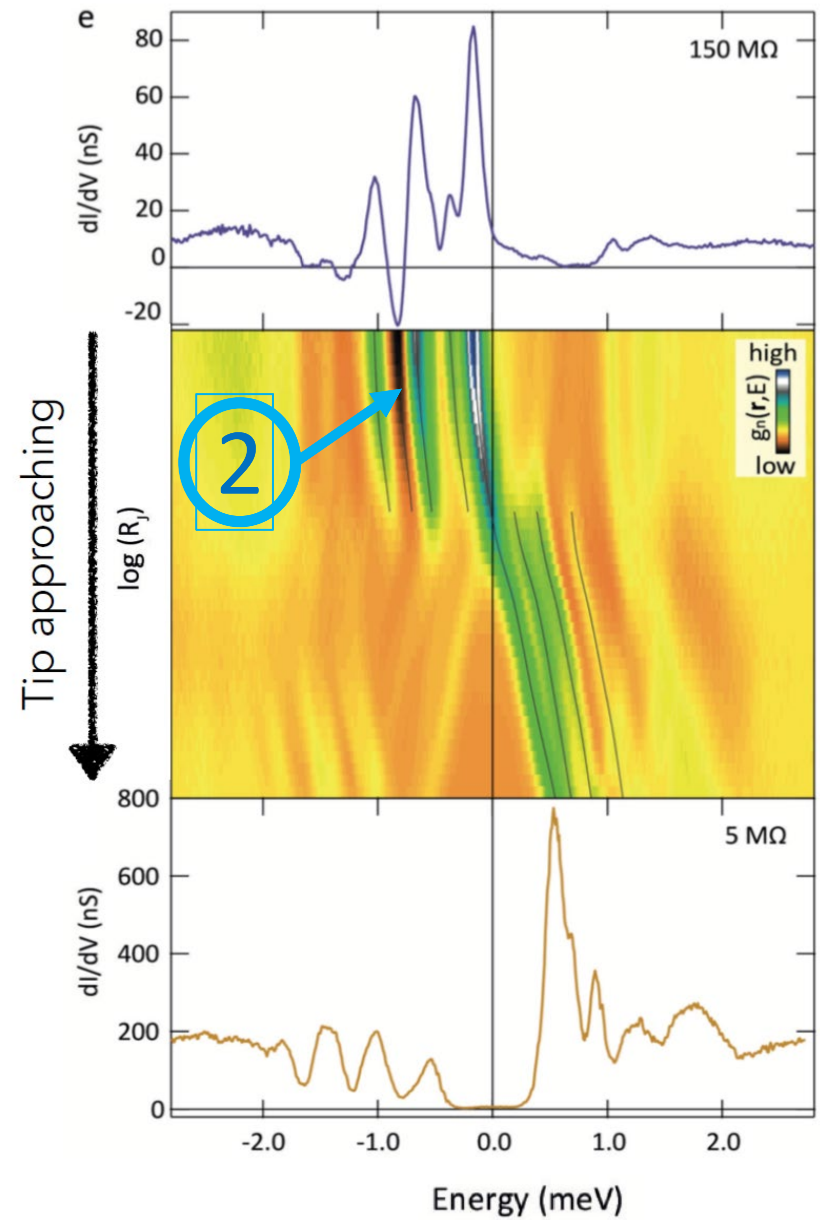
Two key features:

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

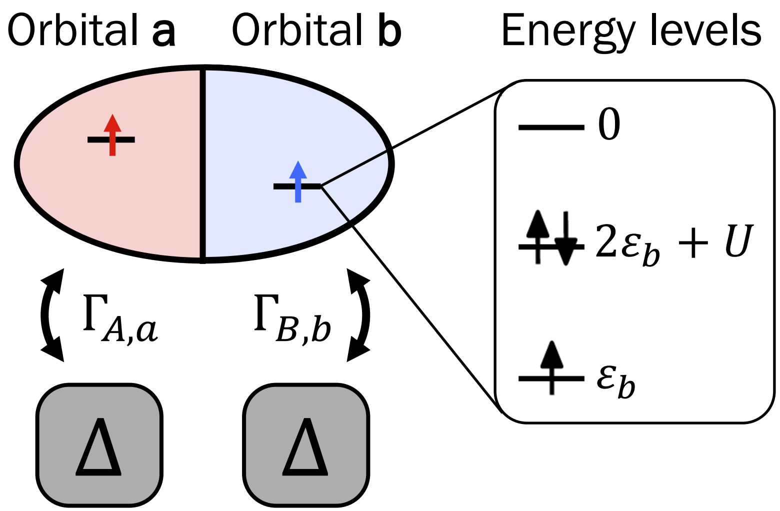
Independent classical YSR channels

2) Appearance of negative differential conductance (NDC)

Multiple impurity states and Coulomb interaction



Multi-channel
Anderson impurity model



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

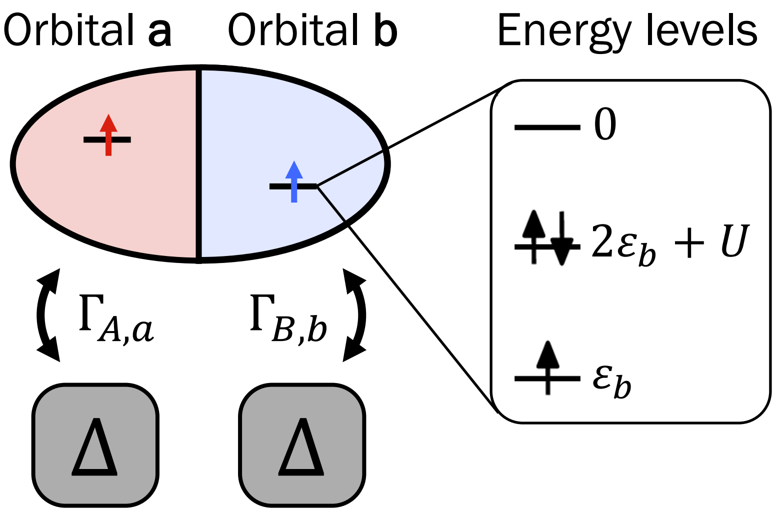
$$H = H_{SC} + H_T + H_{imp}$$

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

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

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

Multi-channel Anderson impurity model



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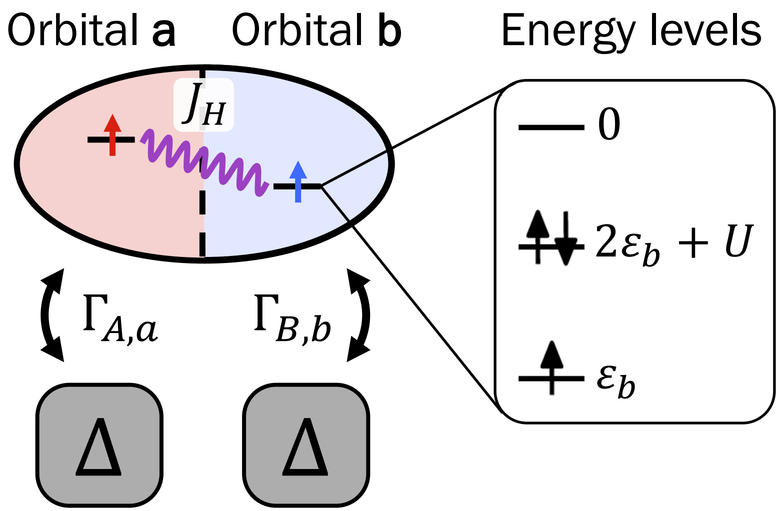
$$\bar{\varepsilon} = \frac{\varepsilon_a + \varepsilon_b}{2}$$

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

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

Multi-channel Anderson impurity model



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

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

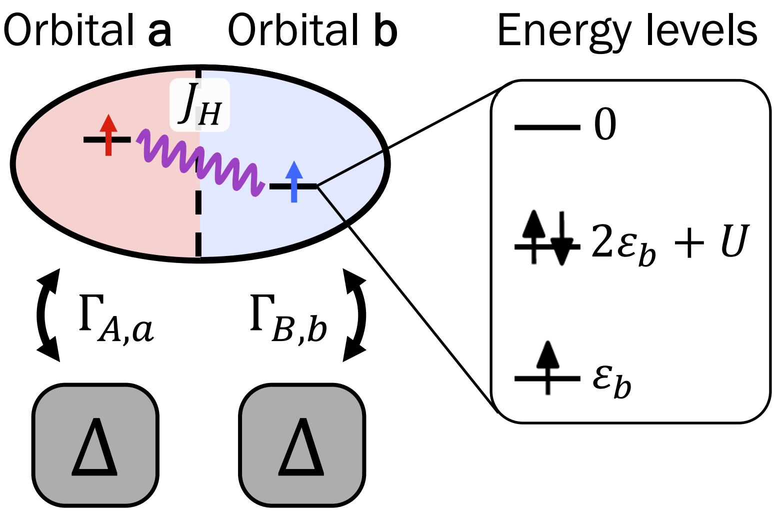
Hund's coupling
$J_H > 0$

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

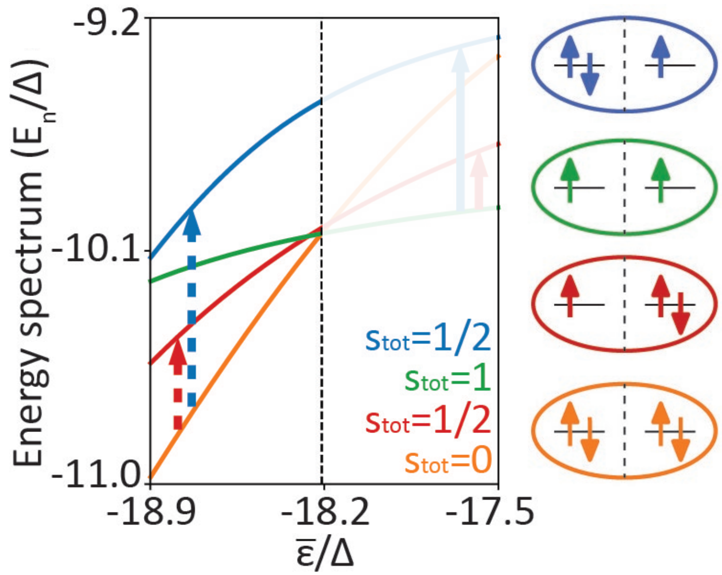
'crystal field' splitting $\delta\varepsilon = \varepsilon_a - \varepsilon_b = \mathrm{C}$

$\bar{\varepsilon}$ 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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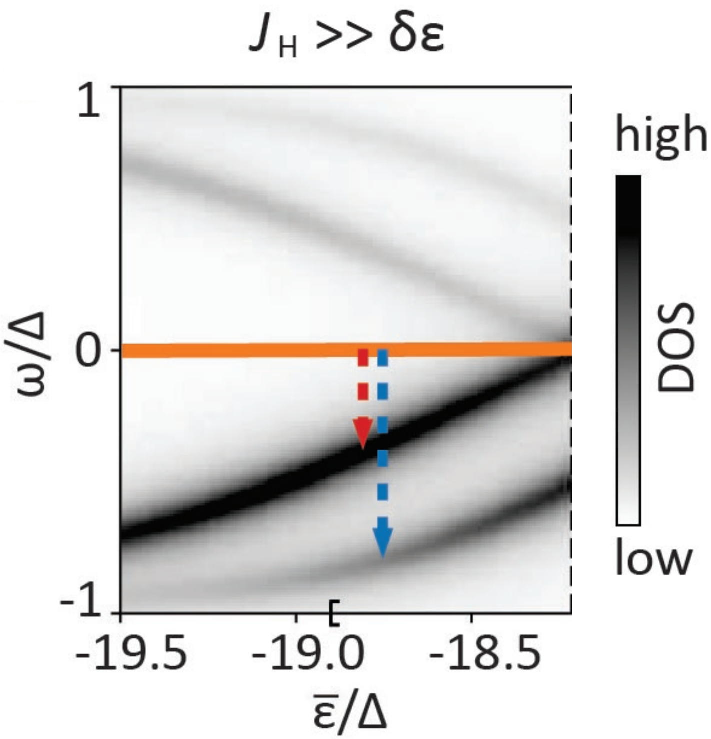
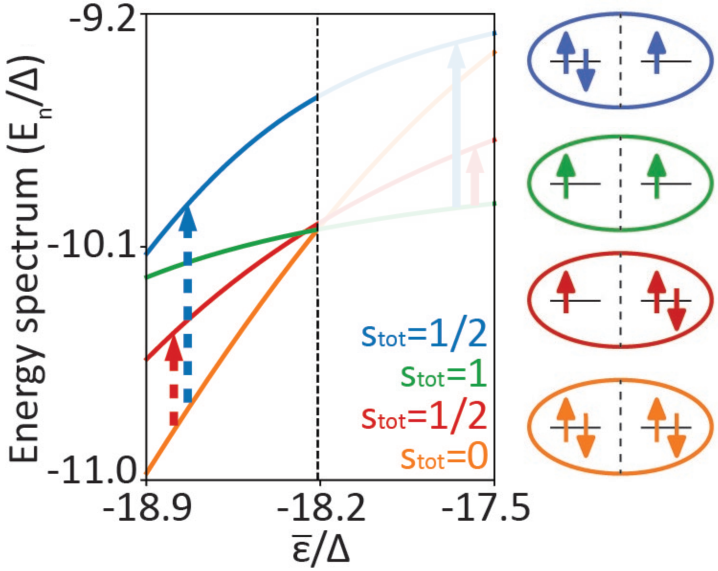
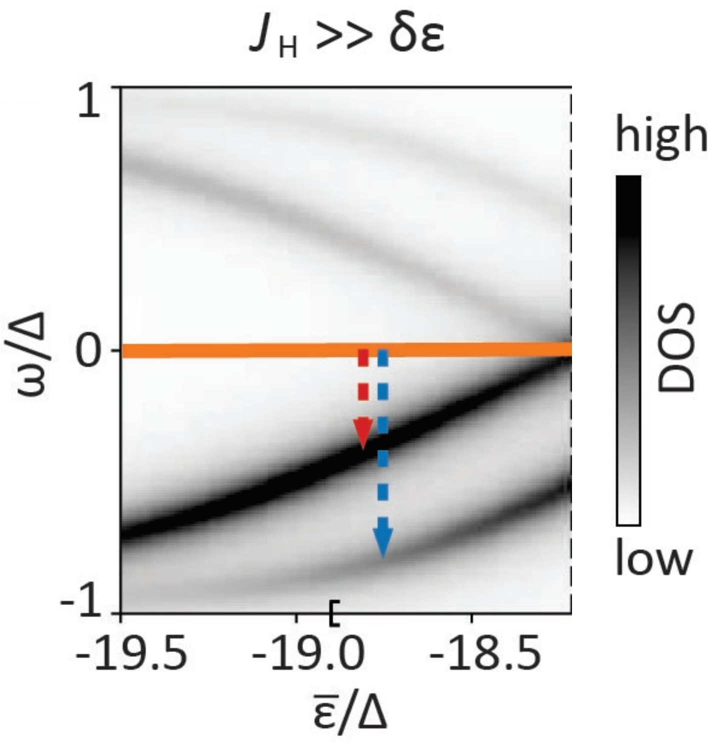
Multi-channel Anderson impurity model: many-body spectrum

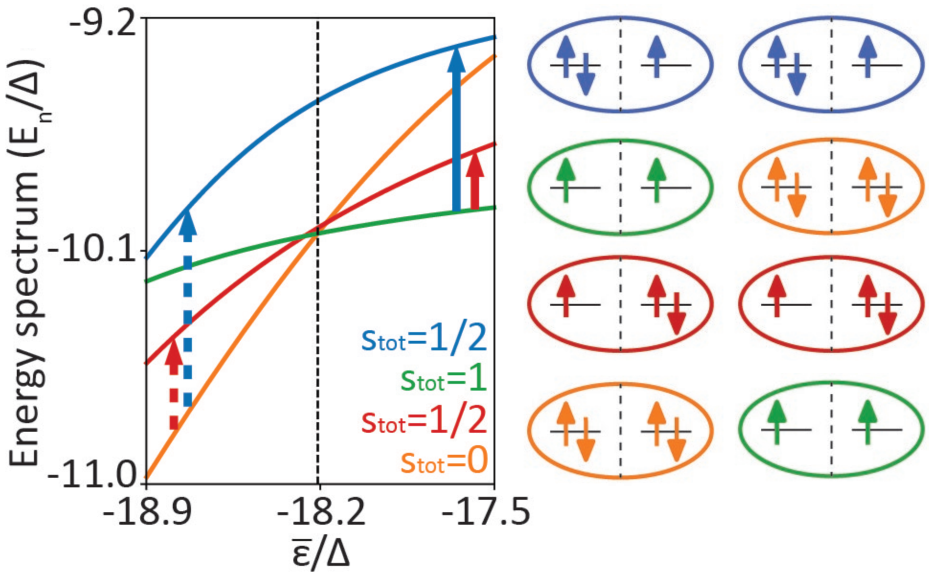




M. Uldemolins et al., Nature Comm 15, 8526 (2024)

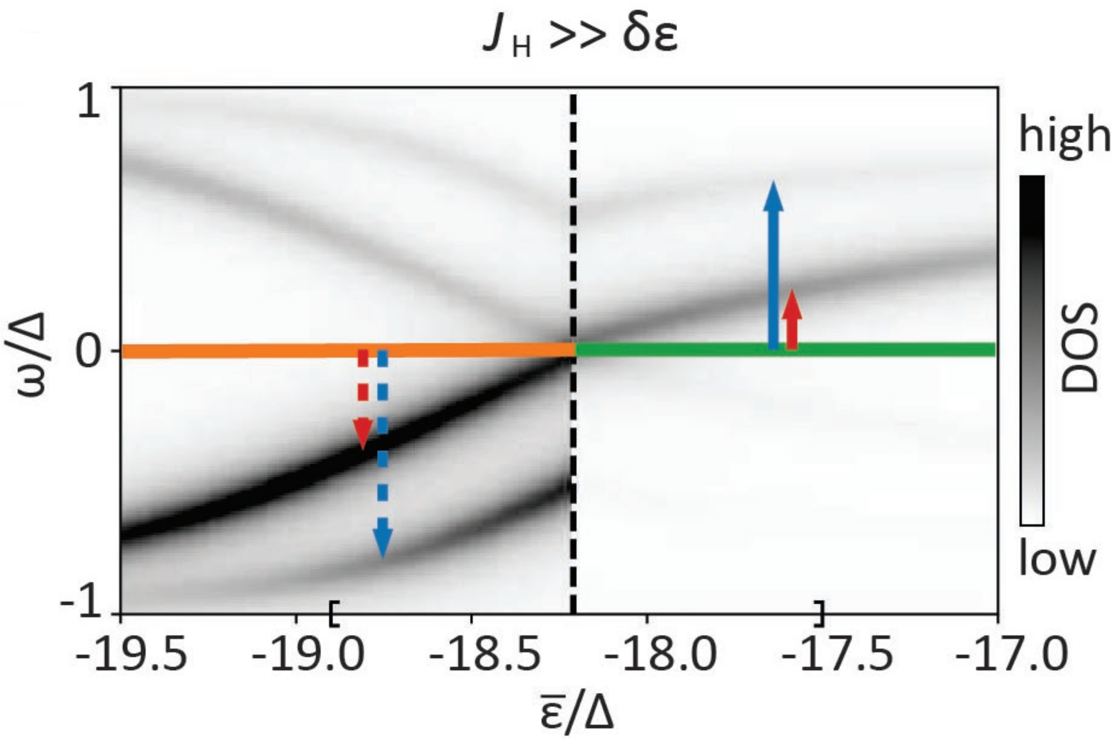
Multi-channel
Quantum phase transition

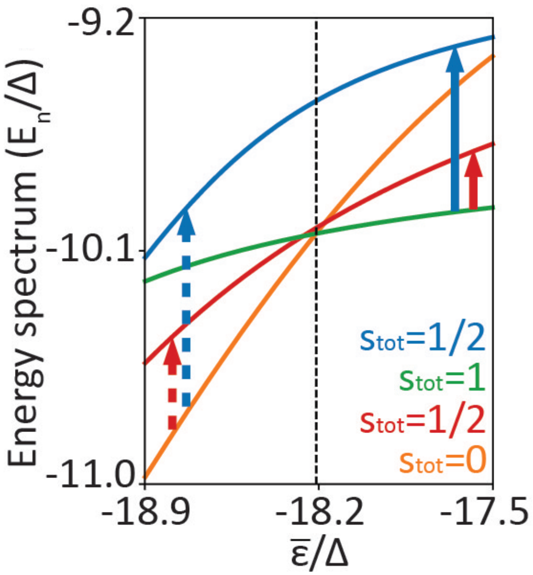




- Multi-channel quantum phase transition: large change in occupation
- Orbital energy cost compensated by gain of Hund's energy

Multi-channel
Quantum phase transition

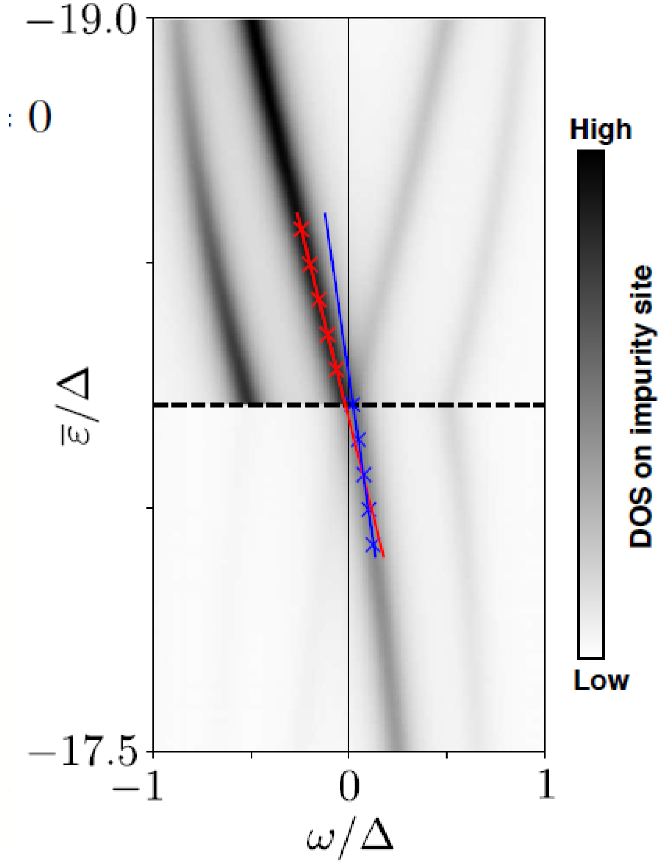


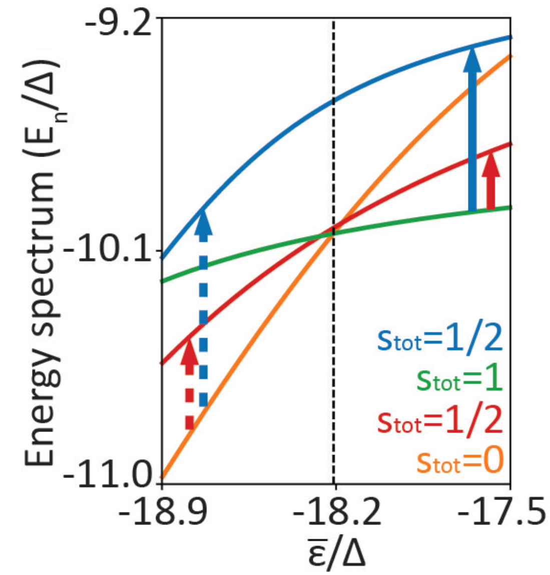


- ➢ Calculated LDOS captures STM experiment

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

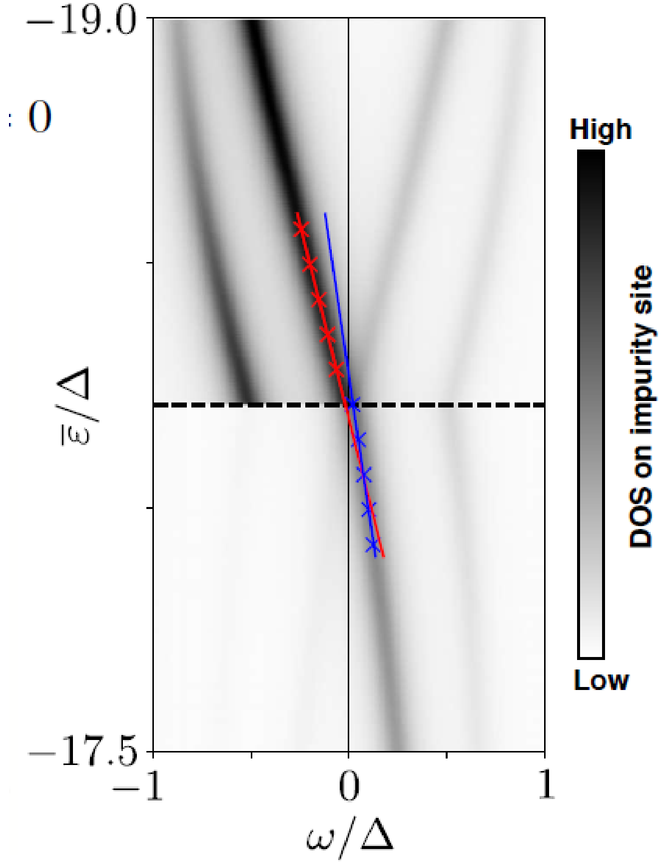
Slope changes upon crossing E=0

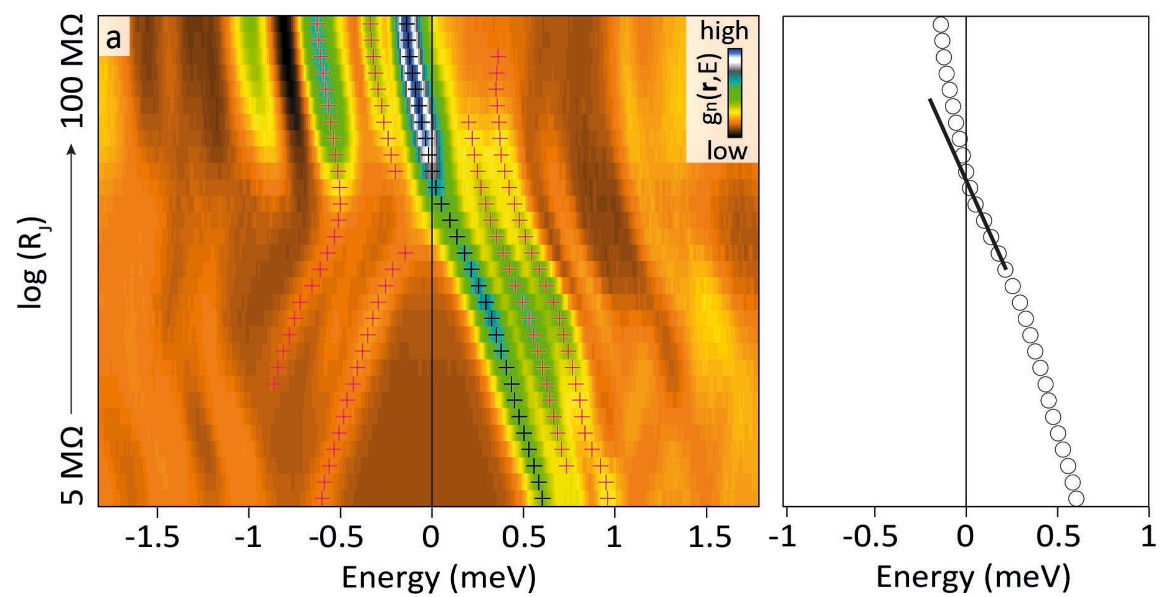




- Discontinuous slope at E = 0

Slope changes upon crossing E=0

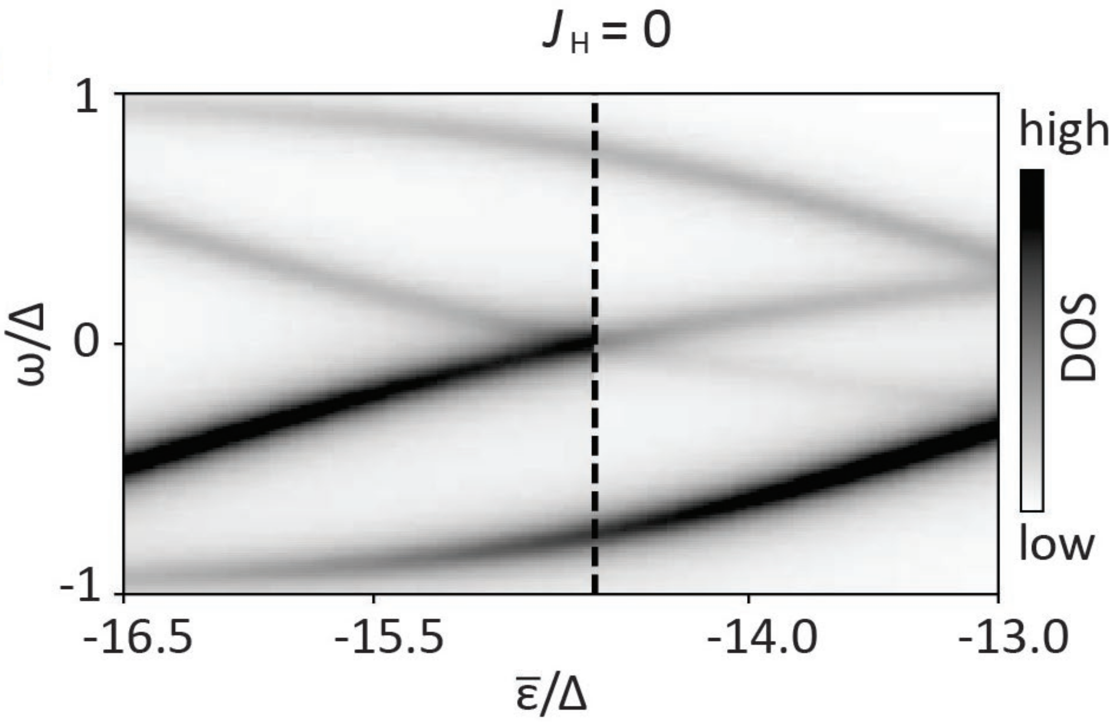




- Discontinuous slope at E = 0

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)

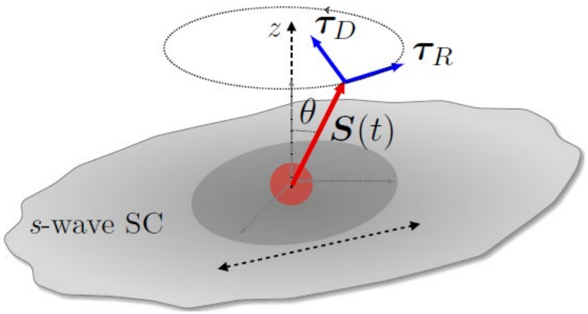
Multi-channel quantum phase transition (MCQPT)

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 properties of YSR states?

Spin precessing classical magnetic impurity



$$H_{\text{imp}} = -J\boldsymbol{S}(t)\cdot\boldsymbol{\sigma}\delta(\mathbf{r})$$

$$\boldsymbol{S}(t) = S(\sin\theta\cos\Omega t,\ \ \sin\theta\sin\Omega t,\ \ \cos\theta)$$

Question: Feedback effect of bound electrons on the classical spin dynamics ?

Dynamics of magnetic impurity described by Landau Lifshitz Gilbert Equation:

$$\dot{\boldsymbol{S}}(t) = -\boldsymbol{S}(t)\times\Big(\gamma\boldsymbol{B}(t) - \langle\boldsymbol{\sigma}(t)\rangle + \beta\dot{\boldsymbol{S}}(t)\Big)$$

Spin precessing classical magnetic impurity

Unitary transformation, $U(t) = \exp(-ib\sigma_z t)$, $b = \Omega/2$

$\downarrow$

back to static problem.

$$\boldsymbol{S}(t) \rightarrow \boldsymbol{S}(0) = S(\sin\theta, 0, \cos\theta)$$

$$H_{\mathrm{rot}} = U^\dagger(t) H_{\mathrm{tot}}(t) U(t) + i\dot{U}^\dagger(t) U(t) = H_{\mathrm{tot}}(0) - b\sigma_z$$

Zeeman splitting like term

- General Solution: its complicated
- Adiabatic ($\delta = b/\Delta \ll 1$) and Deep Shiba limit ($\alpha \rightarrow 1$),

$$E_s = E_0 - b\cos\theta$$

Spin precessing classical magnetic impurity

Dynamical reactive torque:

YSR occupation

$$\boldsymbol{\tau}_R(t) = JS\boldsymbol{n} \times \langle \boldsymbol{\sigma} \rangle = \underbrace{\left(n_s - \frac{1}{2}\right)}_{\text{}} \frac{\Omega}{2} \boldsymbol{n} \times \boldsymbol{z}$$

Universal reactive torque independent of the superconductor
(**obtained in the adiabatic and deep Shiba limit**)

Resonance frequency shift due to the Shiba state:

$$\Omega_R = \frac{\Omega_0}{1 + \left(n_S - \frac{1}{2}\right)\frac{1}{2S}}$$

➡ Parity read-out

Mishra et. al., PRB 103, L121401 (2021)

Toward a YSR qubit

Road Map:

Single YSR state →YSR qubit - - - - - - - - - - - - - - → TQC

Manipulating a YSR state

Issue: Parameters hard to control

$\downarrow$

Solution: Dynamics of magnetic impurities

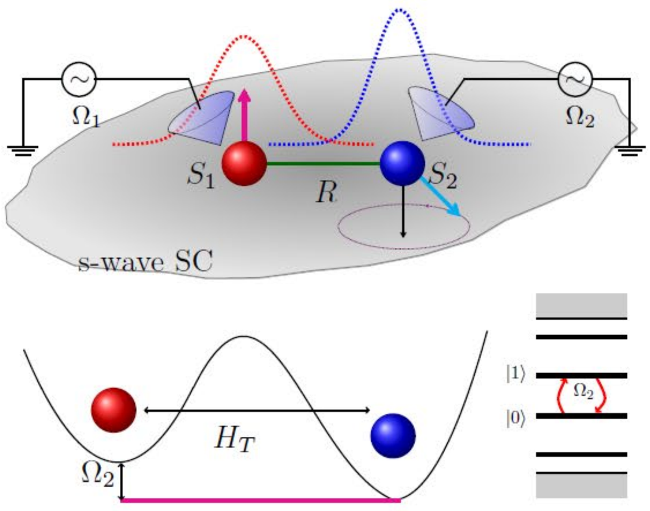
$\downarrow$

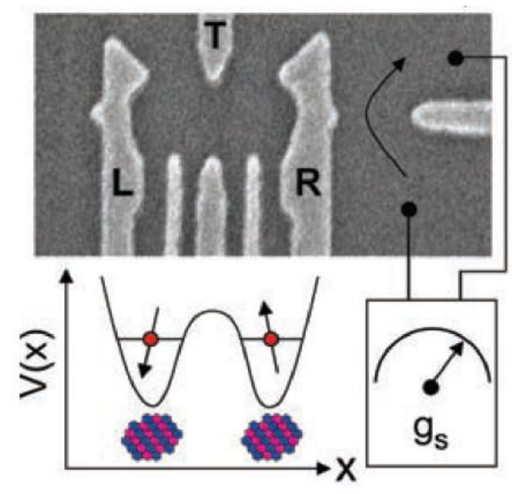
Control knob: Precession frequency

Main message: Dynamics of magnetic impurities to control, manipulate and read out YSR qubit

Kaladzhyan et. al., PRB, 95, 195403 (2017)
Kaladzhyan et. al., PRB, 96, 020507(R) (2017)
Mishra et. al., PRB, 103, L121401 (2021)

Building a YSR qubit





YSR qubit

Petta et. al., Science 309,2180 (2005)

Crux of YSR qubit proposal:

- Dynamics of the spin biases the double well potential $\leftrightarrow$ voltage bias in double quantum dots
- Frequency shift (back action on the spin): occupation of in-gap states $\leftrightarrow$ quantum non-demolition read out in cavity QED setups.

Mishra et. al., PRX Quantum 2, 0403247 (2021)

Summary of the YSR qubit

- Building YSR qubit from Shiba dimer
- Read out and control of qubit via dynamics of the impurities
- Precession of the spin acts as a bias for the double well potential analogous to the double quantum dots
- Read out via frequency shift: Non-invasive technique
- Using stochastic LLG equation, we estimate the decoherence time for the qubit

Some estimates

YSR Qubit

- Qubit splitting, $\Omega_2 = 0.0394$meV,
- Rabi time period: 8.55ns
- At $\theta = \pi$, relaxation time $T_r = 110$ns.
- Parameters: $\Delta = 1$meV, $R = 2.9\zeta$, $\alpha_1 = 1.15$, $\alpha_2 = 1.1$, $\theta = \pi - 0.1$, $\alpha_g = 0.001$.

Andreev Qubit

- Rabi time period: $T \approx 20$ns
- Relaxation time $T_r = 4\mu$s
- Phase difference, $\delta = \pi$

Janvier et.al. Science 349,1199 (2015)