



Yu-Shiba-Rusinov states in real metals

Felix von Oppen
Freie Universität Berlin

Kondo effect in real metals

Ph. Nozières

Institut Laue-Langevin, 156X, 38042 Grenoble Cedex, France

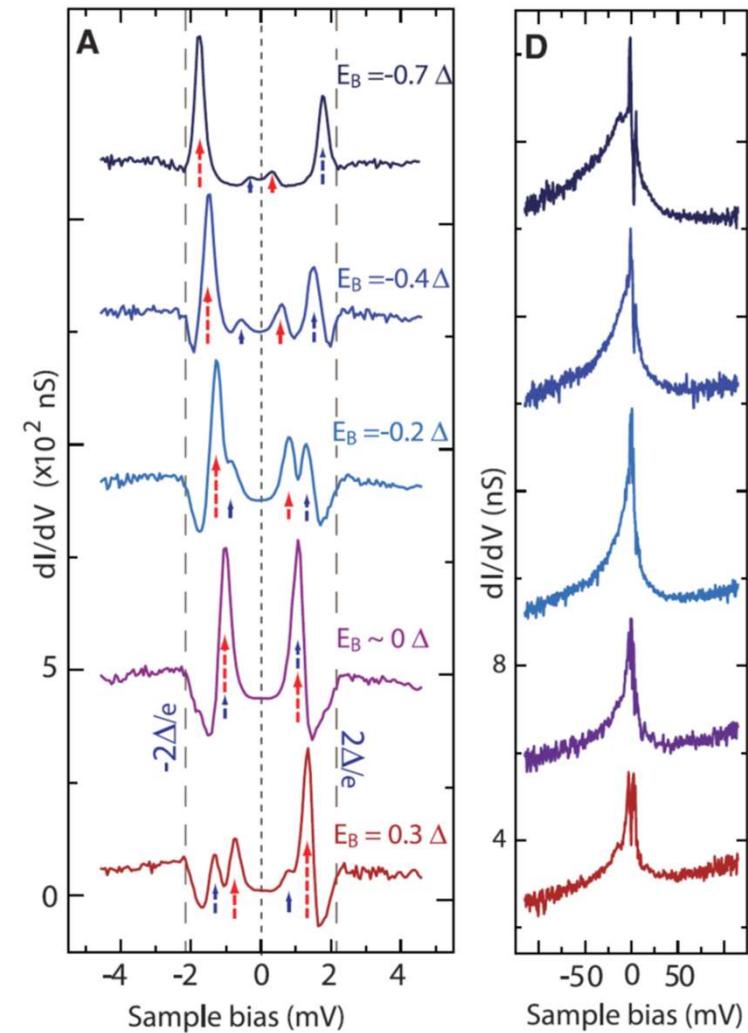
and A. Blandin

Laboratoire de Physique des Solides, Université Paris-Sud, 91405 Orsay, France

(*Reçu le 21 septembre 1979, accepté le 30 octobre 1979*)

higher spins & multiple channels

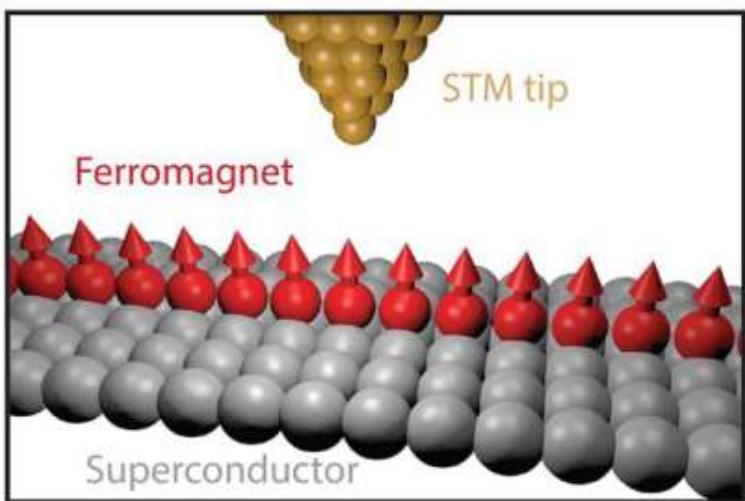
- exchange coupling
- crystal fields
- magnetic anisotropy
- ...
- quantum spins



MnPc on Pb(111)

Franke et al., Science 2011

Novel quantum phases



Yazdani group, Science (2014)

see also:

Ruby et al., PRL (2015)

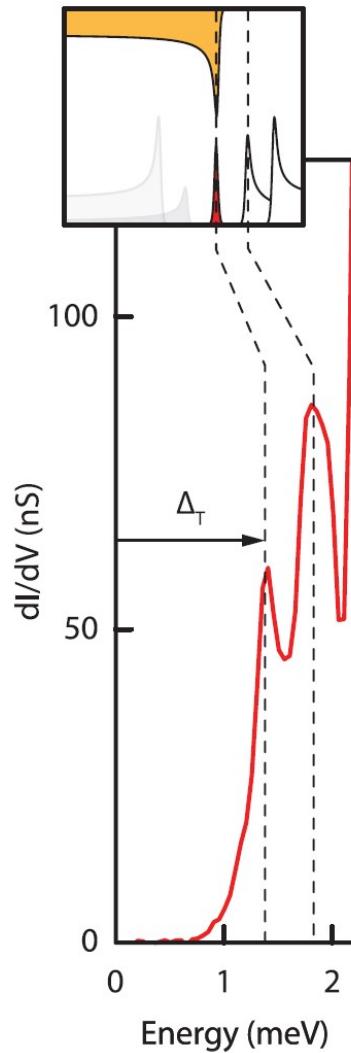
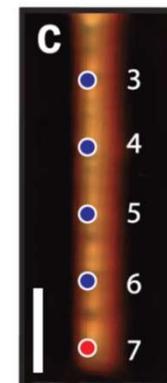
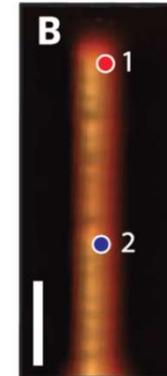
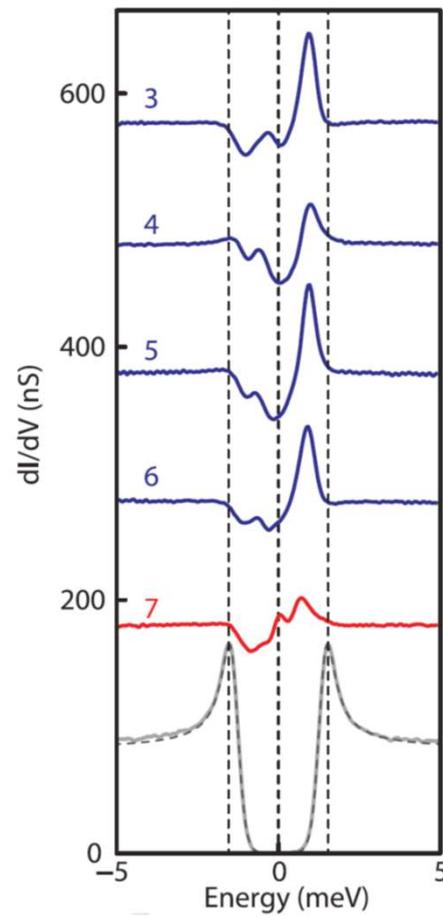
Pawlak et al., npj QI (2016)

Feldman et al., Nat. Phys. (2017)

Jeon et al., Science (2017)

Kim et al., Sci. Adv. (2018)

...



Fe adatoms on Pb(110)



Wave-Function Hybridization in Yu-Shiba-Rusinov Dimers

PRL 2018

Michael Ruby,¹ Benjamin W. Heinrich,¹ Yang Peng,^{2,3,4} Felix von Oppen,² and Katharina J. Franke¹

Mn on Pb

Coupled Yu–Shiba–Rusinov States in Molecular Dimers on NbSe₂

Shawulienu Kezilebieke,[†] Marc Dvorak,[‡] Teemu Ojanen,^{*,†} and Peter Liljeroth^{*,†} Nano Lett. 2018

CuPc on
NbSe₂

Influence of Magnetic Ordering between Cr Adatoms on the Yu-Shiba-Rusinov States of the β -Bi₂Pd Superconductor

Deung-Jang Choi,^{1,2,3,4,*} Carlos García Fernández,² Edwin Herrera,⁵ Carmen Rubio-Verdú,³ Miguel M. Ugeda,^{1,4}
Isabel Guillamón,⁵ Hermann Suderow,⁵ José Ignacio Pascual,^{3,4} and Nicolás Lorente^{1,2} PRL 2018

Tuning interactions between spins in a superconductor

Hao Ding (丁浩)^{a,b,1}, Yuwen Hu^{a,b,1}, Mallika T. Randeria^{a,b,2}, Silas Hoffman^{c,d}, Oindrila Deb^c, Jelena Klinovaja^c,
Daniel Loss^c, and Ali Yazdani^{a,b,3} PNAS 2021

Long range and highly tunable interaction between local spins coupled to a superconducting condensate

Nat. Comm. 2021

Felix Küster¹, Sascha Brinker¹, Samir Lounis^{2,3}, Stuart S. P. Parkin¹ & Paolo Sessi¹

Quantum spins and hybridization in artificially-constructed chains of magnetic adatoms on a superconductor

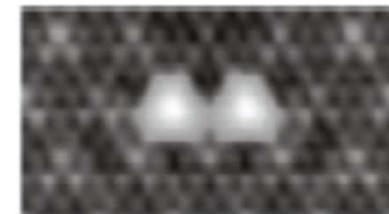
Nat. Comm. 2022

Eva Liehaber¹, Lisa M. Rütten¹, Gaël Reecht¹, Jacob F. Steiner¹, Sebastian Rohlf³, Kai Rossnagel^{3,4},
Felix von Oppen² & Katharina J. Franke¹

Cr on Bi₂Pd

Gd on Bi/Nb

Cr on Nb



Fe on NbSe₂

Outline



- YSR in real metals:
monomers & dimers
- Adatom chains: quantum
magnetism & topological
superconductivity
- Diode effect in YSR
Josephson junctions

- *YSR states in real metals*
FvO & K. Franke
PRB **103, 205424 (2021)**
- *Quantum magnetism topological
superconductivity in YSR chains*
J. Steiner, C. Mora, K. Franke, FvO,
PRL **128, 036801 (2022)**
- *Quantum Yu-Shiba-Rusinov dimers*
H. Schmid, J. Steiner, K. Franke, FvO
PRB **105, 235406 (2022)**
- *Quantum spins and hybridization in
chains of magnetic adatoms on a SC*
E. Liebhaber, ..., FvO, K. Franke
Nature Comm. **13, 2160 (2022)**
- *Diode behavior in JJs w/ magnetic atom*
M. Trahms, ..., FvO, K. Franke



Jacob Steiner



Larissa
Melischek



Harald Schmid



Christophe Mora



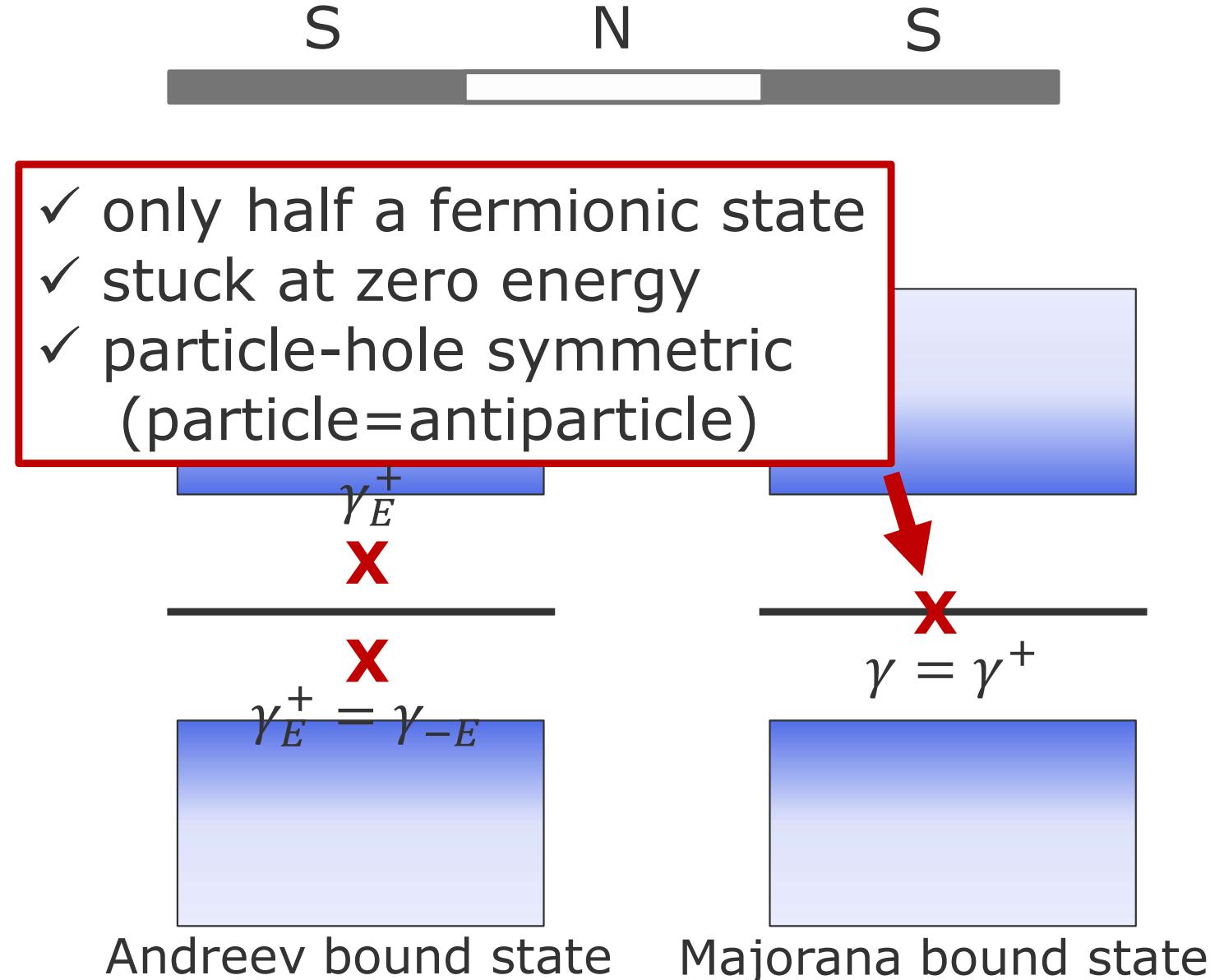
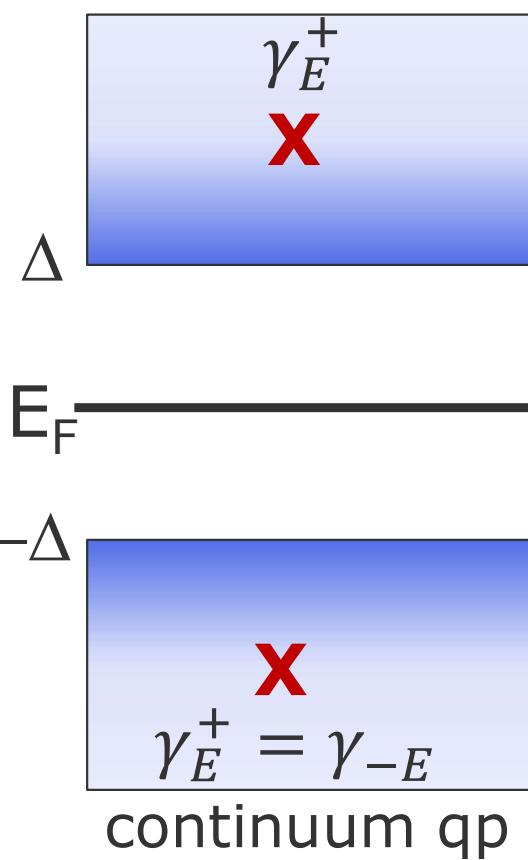
Martina Trahms



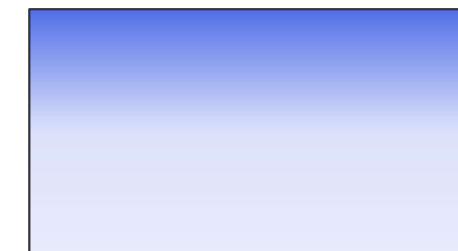
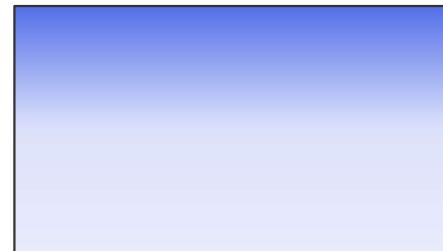
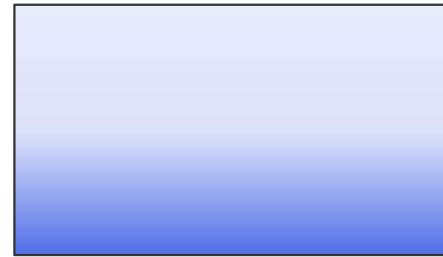
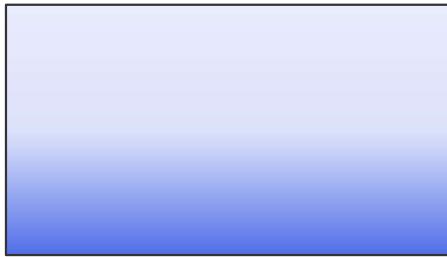
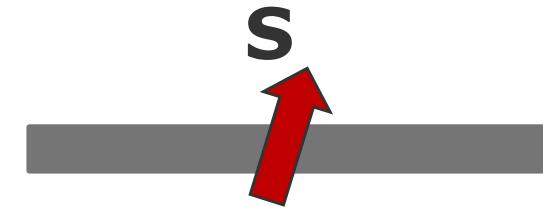
Katharina Franke

Andreev and Majorana states

1D
superconductor



Subgap states in SCs

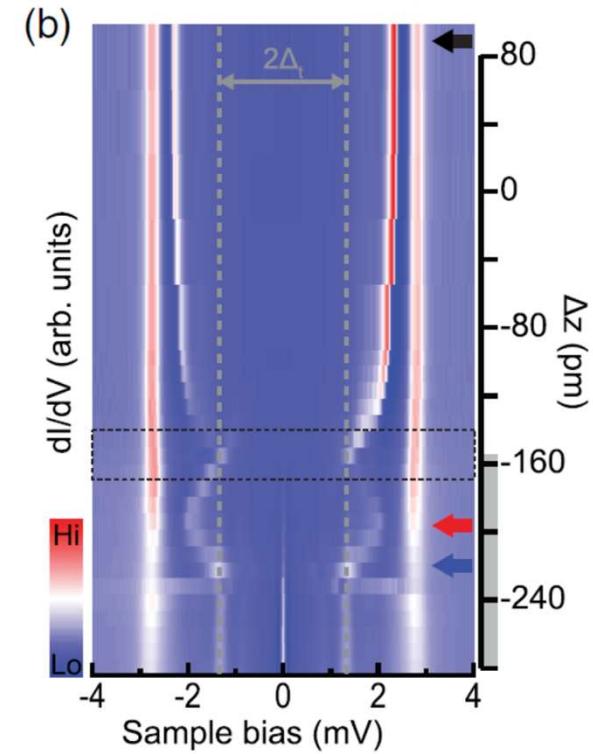
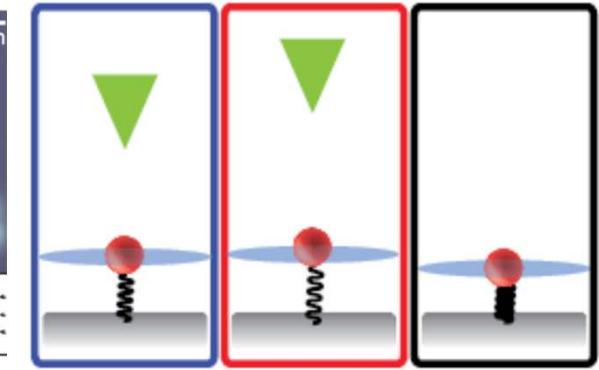
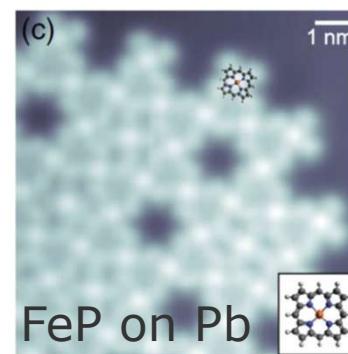
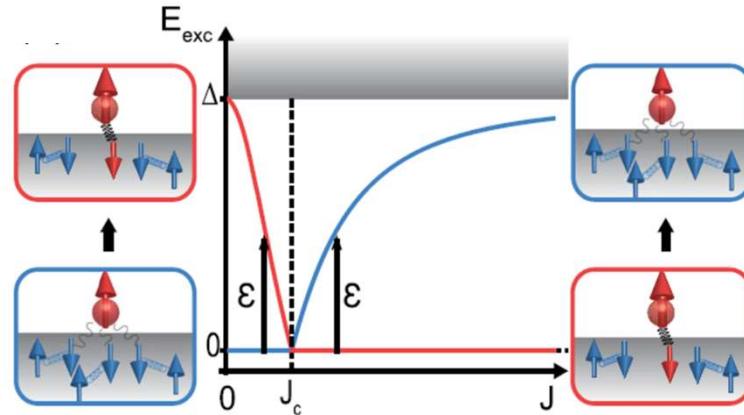
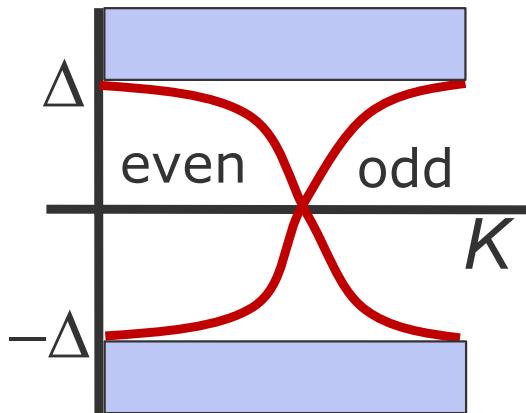


Progress of Theoretical Physics, Vol. 40, No. 3, September 1968

Classical Spins in Superconductors

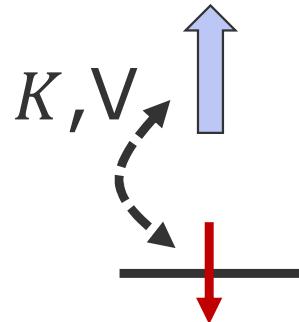
Hiroyuki SHIBA^{*)}

$$H_{sd} = K \sum_{kk'} \psi_{kk'}^\dagger [\sigma_z S_z + \frac{1}{2} (\sigma_+ S_- + \sigma_- S_+)] \psi_{k'}$$



Farinacci, .. FvO, Franke, PRL 2018

Screening



$$H = \Delta(c_{\uparrow}^+ c_{\downarrow}^+ + \text{h. c.}) + \sum_{\sigma\sigma'} c_{\sigma}^+ [V\delta_{\sigma\sigma'} + K\mathbf{S} \cdot \mathbf{s}_{\sigma\sigma'}] c_{\sigma'}$$

Even fermion parity:

Odd parity (q):

Odd parity (c):

|B

Adatom spin is screened only in the quantum case!

$$|\pm\rangle = |BCS\rangle \otimes |\uparrow/\downarrow\rangle$$

$$E_e = -\sqrt{\Delta^2 + V^2}$$

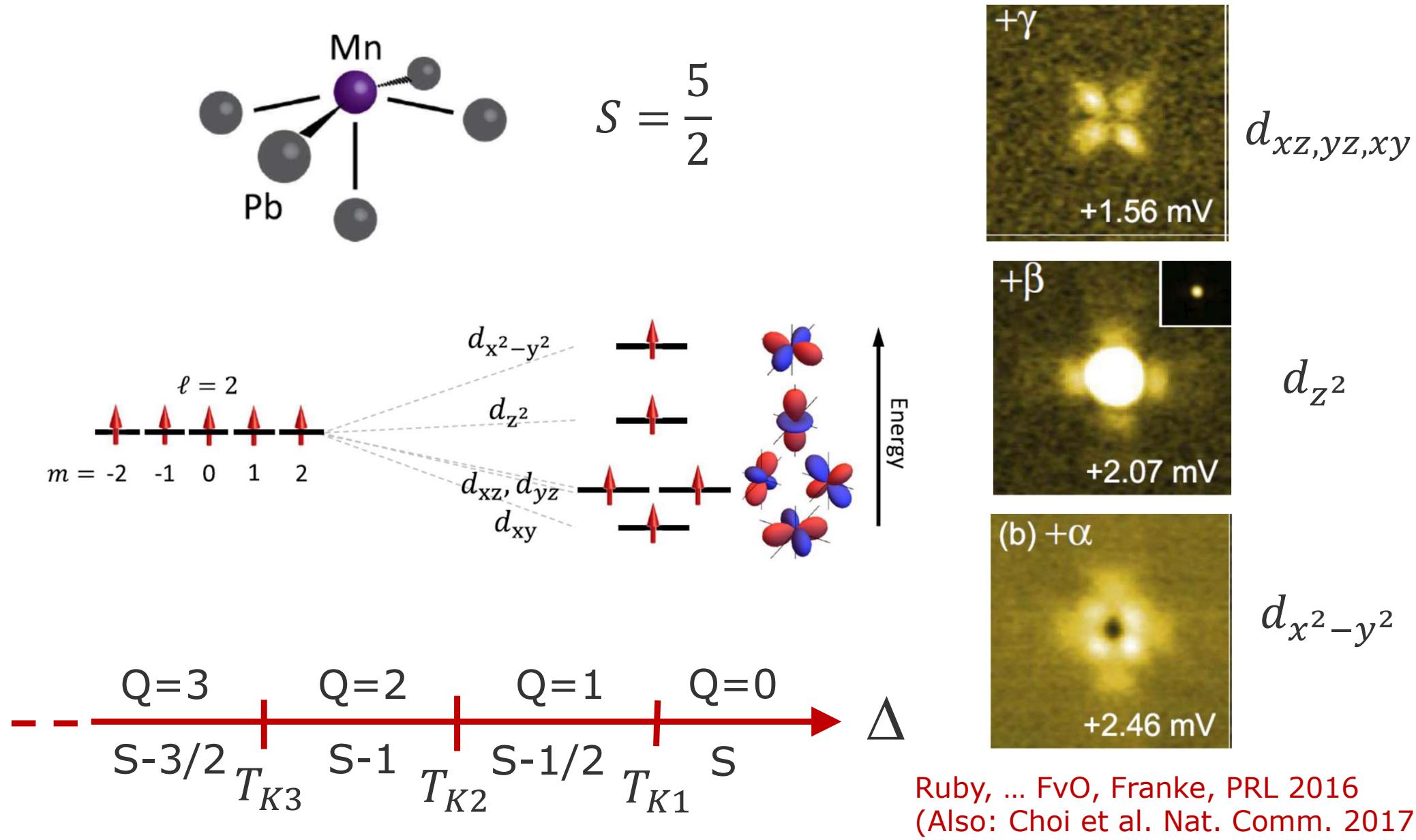
$$|0\rangle = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$

$$E_o = -3K/4$$

$$|0\rangle = |\uparrow\downarrow\rangle \text{ or } |\downarrow\uparrow\rangle$$

$$E_o = -K/4$$

Crystal field effects





$$H = \Delta(c_{\downarrow}^{\dagger}c_{\uparrow}^{\dagger} + c_{\uparrow}c_{\downarrow}) + \sum_{\sigma\sigma'} JS_i \cdot c_{\sigma}^{\dagger} \mathbf{s}_{\sigma\sigma'} c_{\sigma'} + DS_{i,z}^2$$

Easy axis ($D < 0$)

$$\begin{array}{cc} \underline{-1/2} & \underline{1/2} \\ \underline{-3/2} & \underline{3/2} \\ \underline{-5/2} & \underline{5/2} \end{array}$$

Easy plane ($D > 0$)

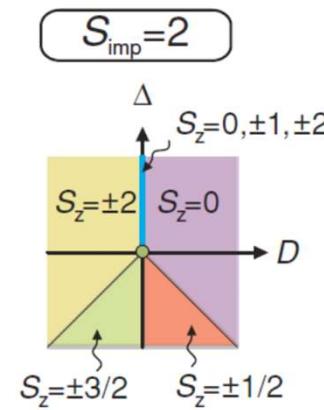
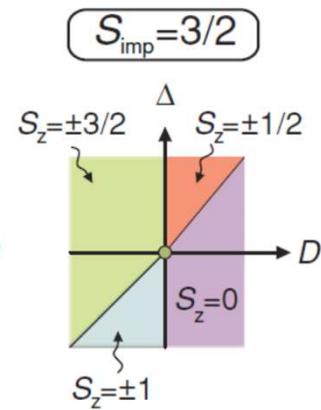
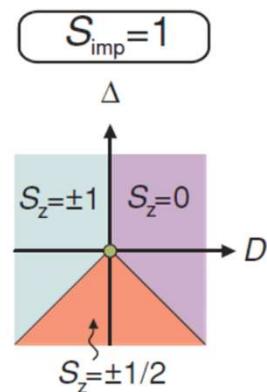
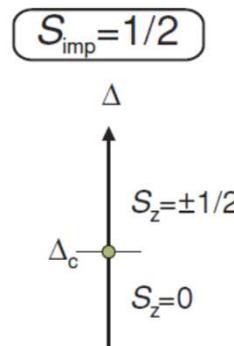
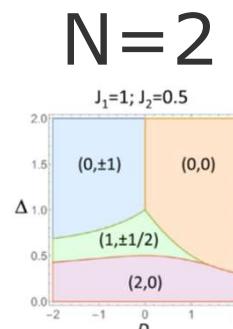
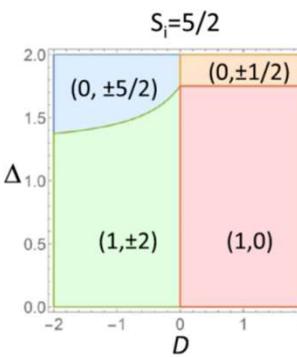
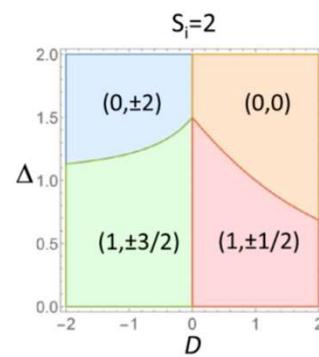
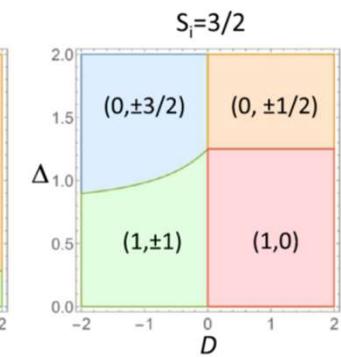
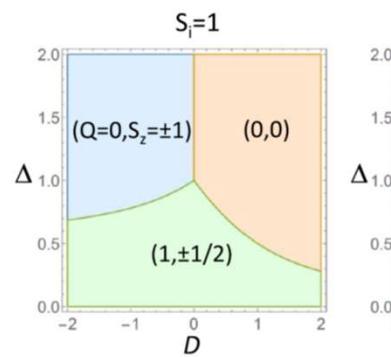
$$\begin{array}{cc} \underline{z/\xi} & \underline{-z/\xi} \\ \underline{z/\varepsilon} & \underline{-z/\varepsilon} \\ \underline{-z/\tau} & \underline{z/\tau} \end{array}$$

- anisotropy frustrates transverse exchange

- importance of Kramers degeneracy

Phase diagrams

ZBM



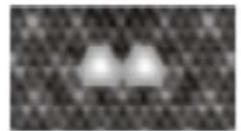
NRG

Zitko et al., PRB 2011

- qualitative agreement, also for excitation spectra
- $D > 0$; half-integer spin: Kondo renormalizations

FvO & K. Franke, PRB **103**, 205424 (2021)

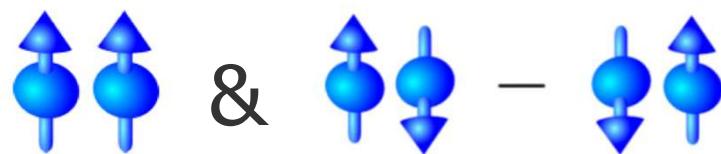
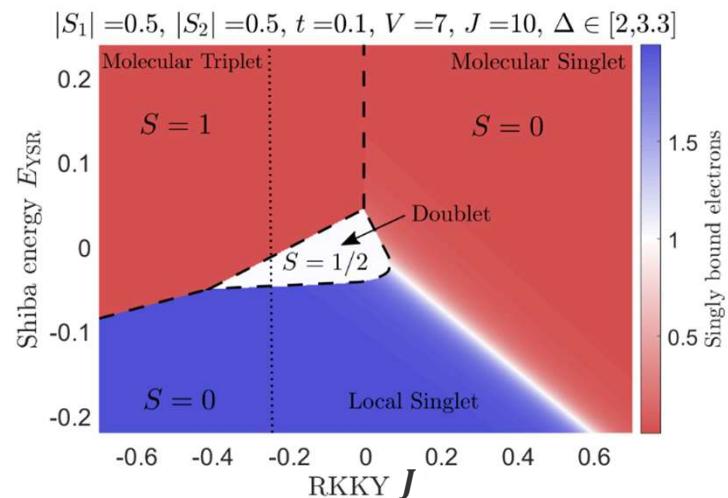
Dimers: Quantum vs classical



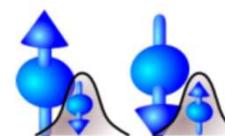
Franke group 2022

$$H = \sum_{j=1}^2 \Delta(c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger + \text{H.c.}) - t[c_{1\sigma}^\dagger c_{2\sigma} + \text{H.c.}] + \sum_{j=1}^2 c_{j\sigma}^\dagger [V\delta_{\sigma\sigma'} + \mathbf{S}_j \cdot \hat{K} \cdot \mathbf{s}_{\sigma\sigma'}] c_{j\sigma'} + \mathbf{S}_1 \cdot \hat{J} \cdot \mathbf{S}_2$$

quantum

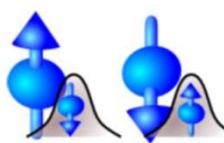
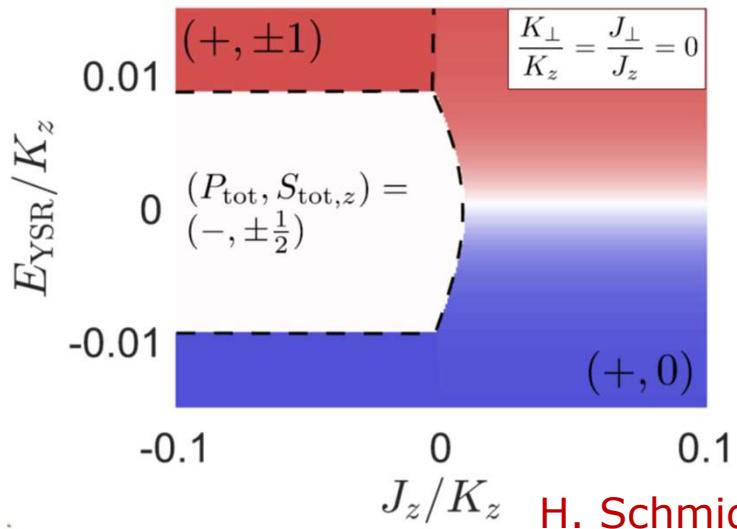


benefit from RKKY energy



does not!

classical

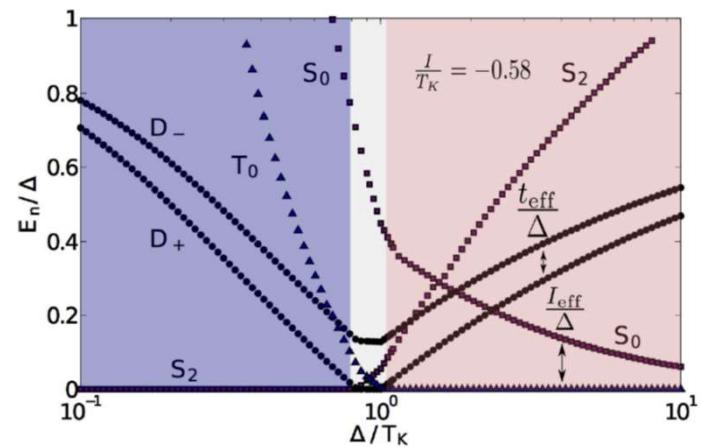
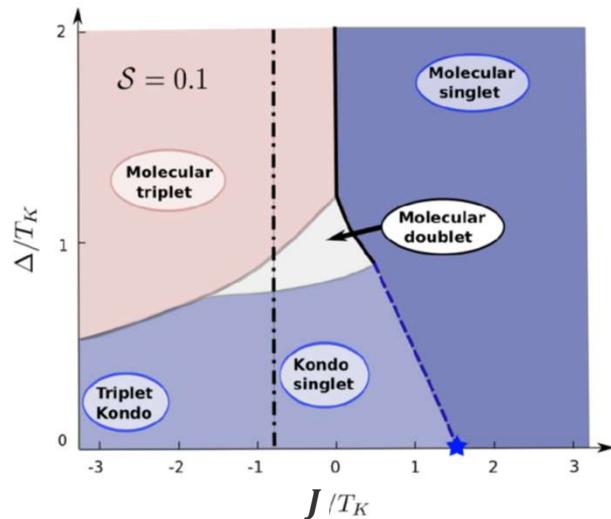


also benefits
from RKKY energy

H. Schmid, J. Steiner, K. Franke, FvO, PRB **105**, 235406 (2022)

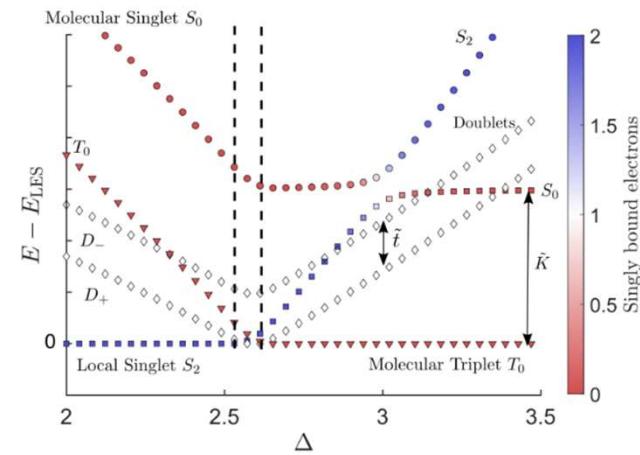
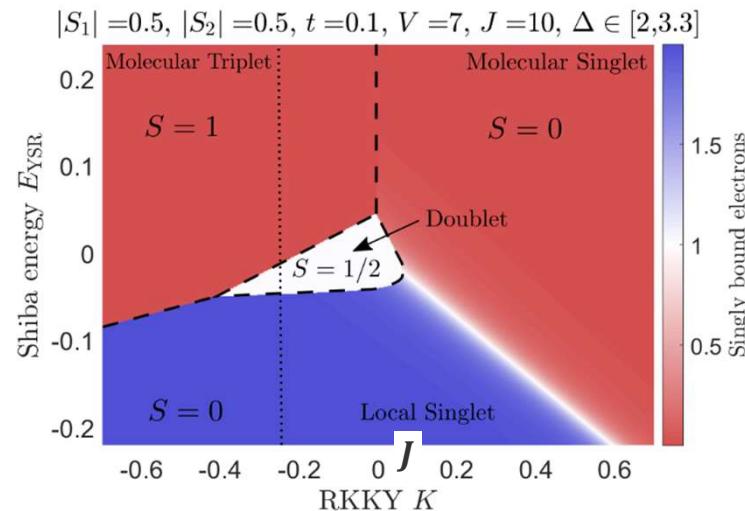
Quantum YSR dimer

NRG



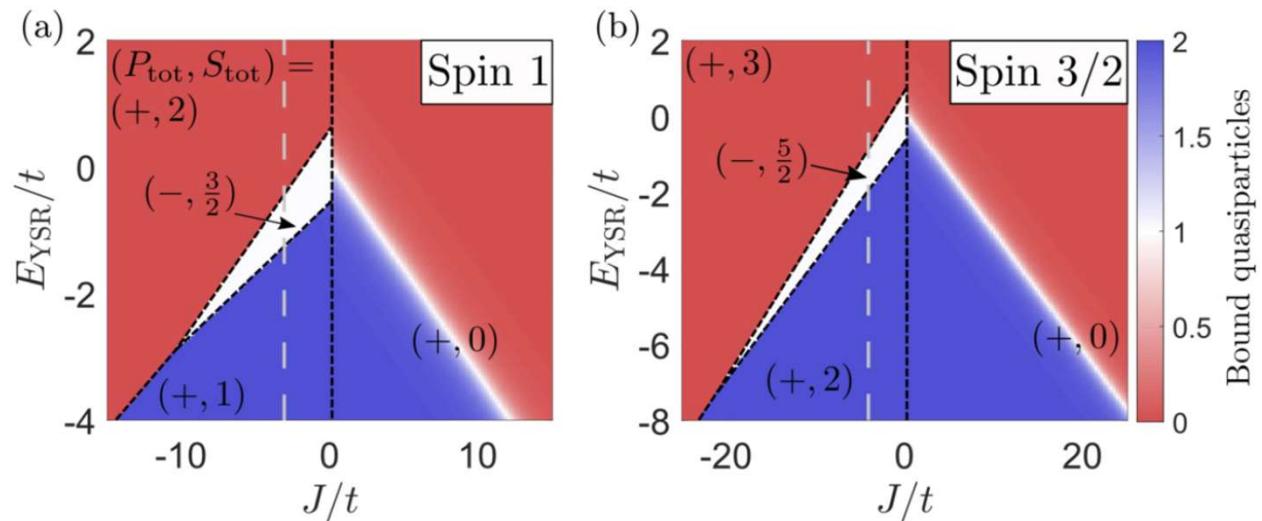
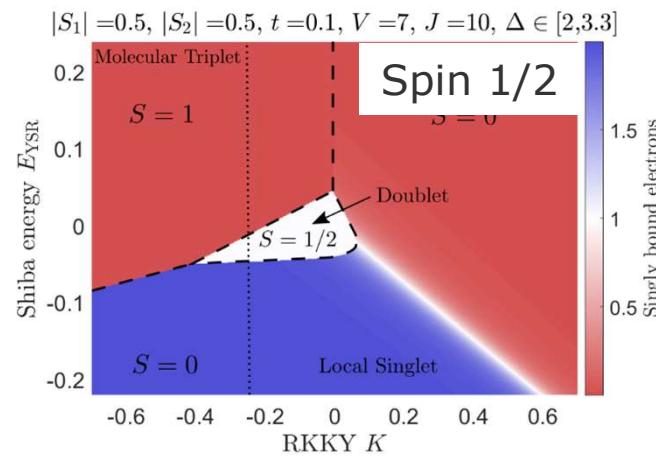
Yao et al., PRB 2014

Zero-bandwidth model



H. Schmid, J. Steiner, K. Franke, FvO, PRB **105**, 235406 (2022)

Large S is not classical

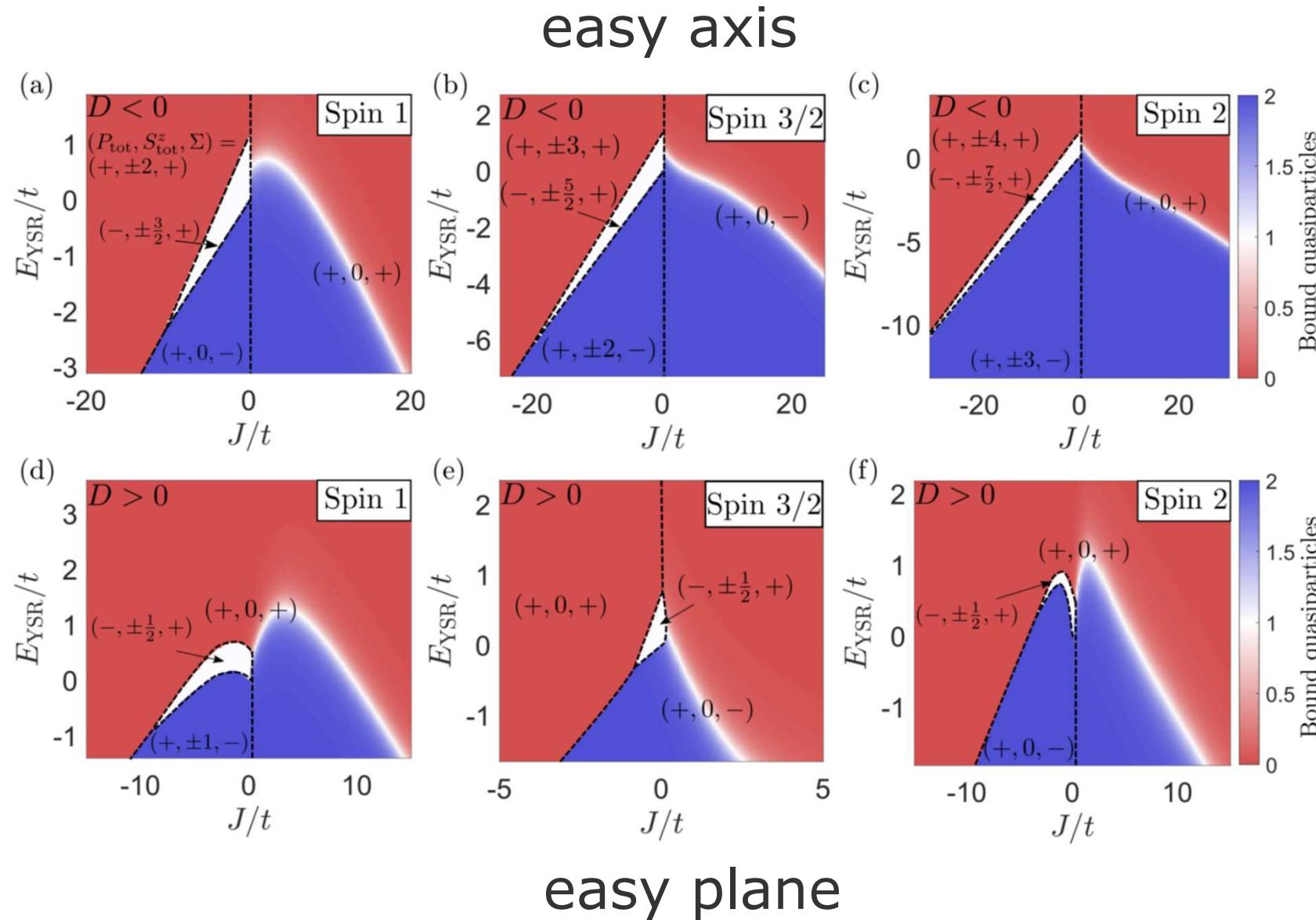


$$J \mathbf{S}_1 \cdot \mathbf{S}_2 \quad \rightarrow \quad E_{\text{RKKY}} = \frac{J}{2} [S_{\text{tot}}(S_{\text{tot}} + 1) - S_1(S_1 + 1) - S_2(S_2 + 1)]$$

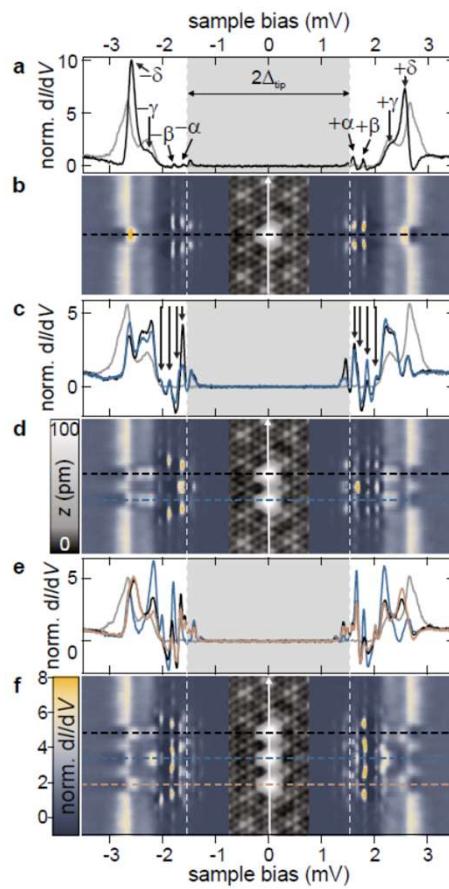
FM phase boundary:
unscreened/
doubly screened

$$E_{\text{YSR}} = \frac{JS}{2S+1} \left(1 - \frac{1}{2S(2S+1)} \right)$$

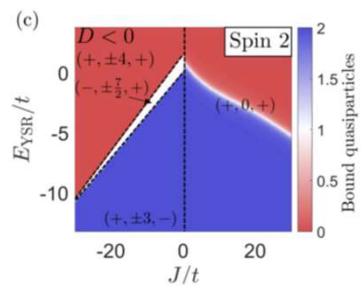
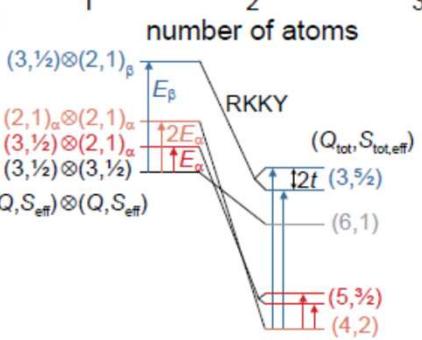
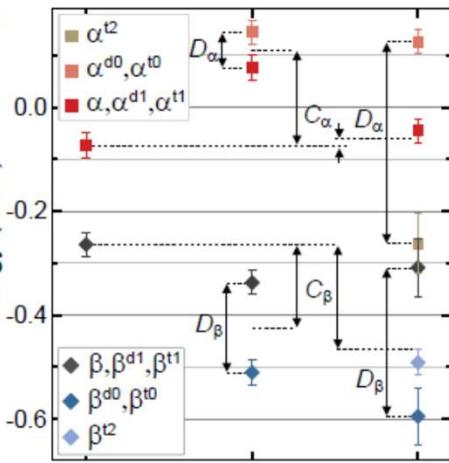
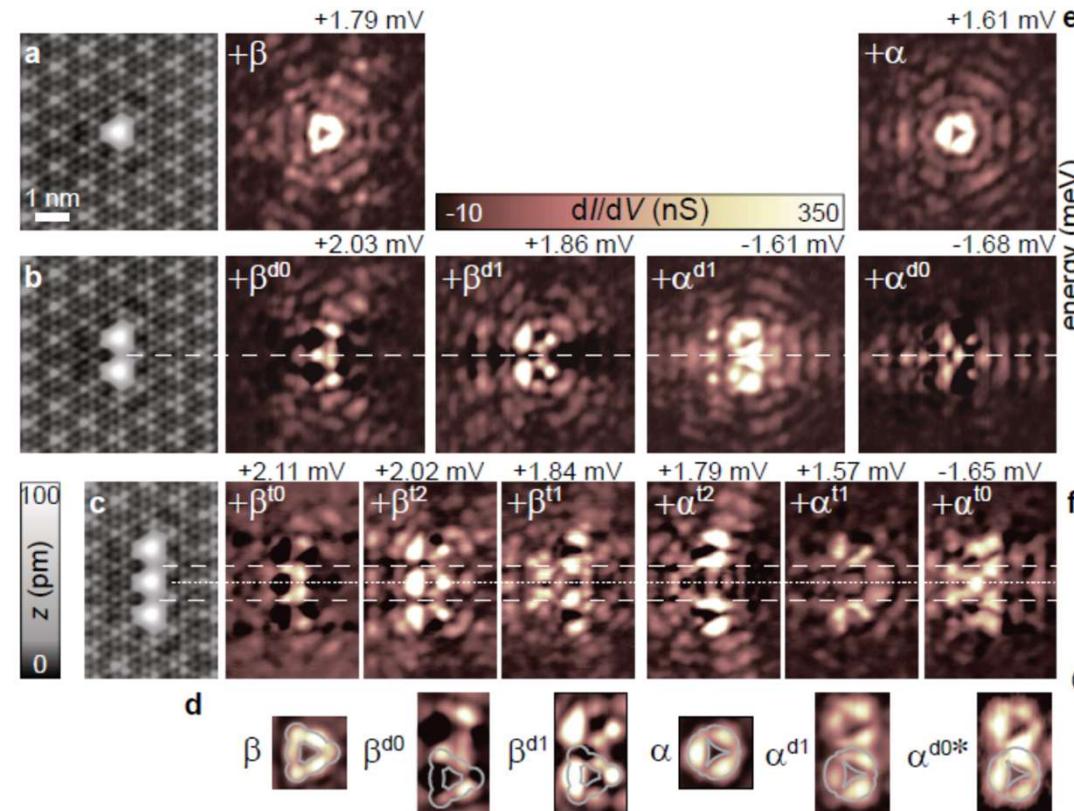
Single-ion anisotropy: not classical!



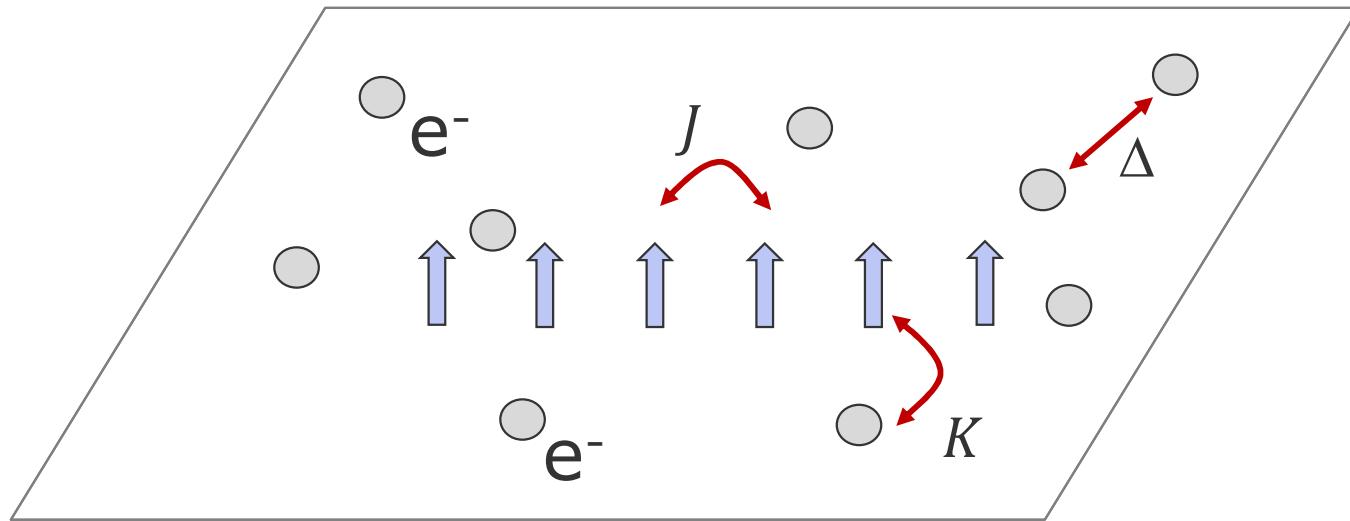
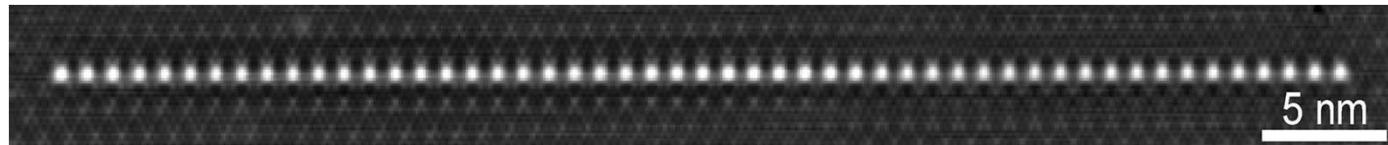
H. Schmid, J. Steiner, K. Franke, FvO, PRB **105**, 235406 (2022)



Fe on NbSe₂



E. Liebhaber, ..., FvO, K. Franke, Nature Comm. 13, 2160 (2022)

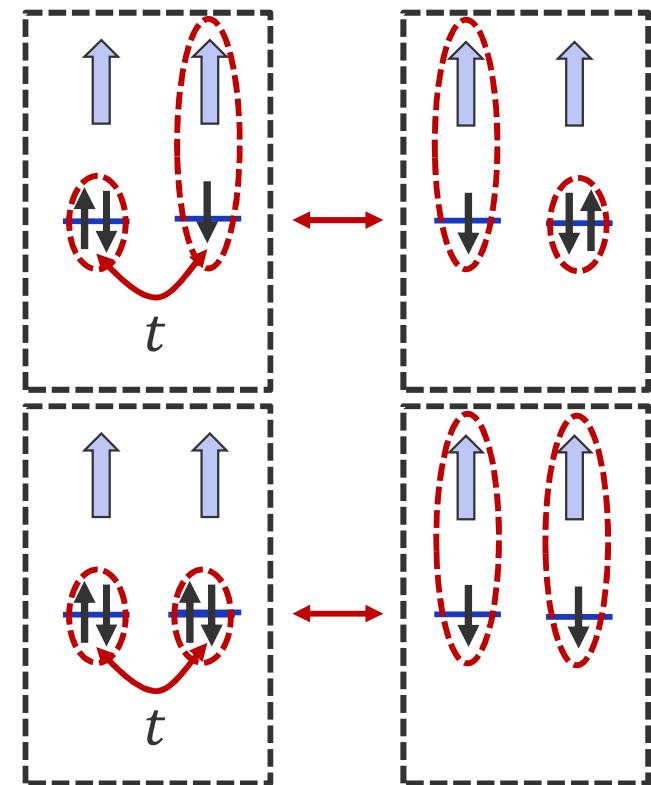
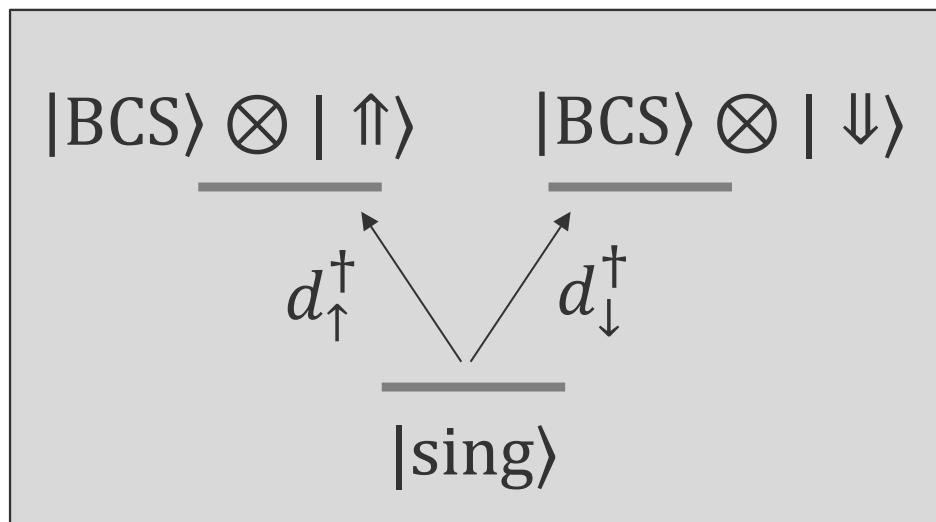
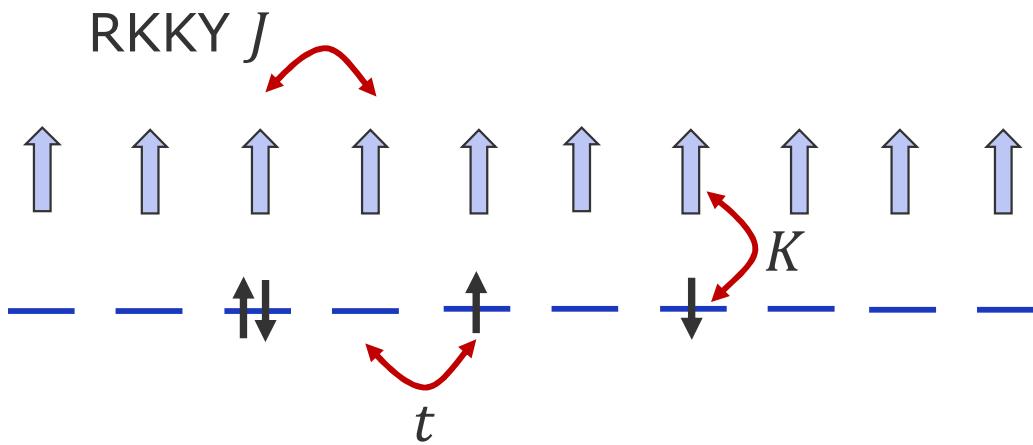


Correlated
spin-fermion
dynamics

- Antiferromagnetic exchange K : Kondo and YSR states
- RKKY interaction J : quantum spin chain
- Electron-electron interactions Δ : superconductivity

$$H = \sum_j \{ \Delta(c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger + \text{H.c.}) + c_{j\sigma}^\dagger [V\delta_{\sigma\sigma'} + \mathbf{S}_j \cdot \mathbf{K} \cdot \mathbf{s}_{\sigma\sigma'} - t[c_{j\sigma}^\dagger c_{j+1,\sigma} + \text{H.c.}] + \mathbf{S}_j \cdot \mathbf{J} \cdot \mathbf{S}_{j+1} + D(S_j^z)^2] \}$$

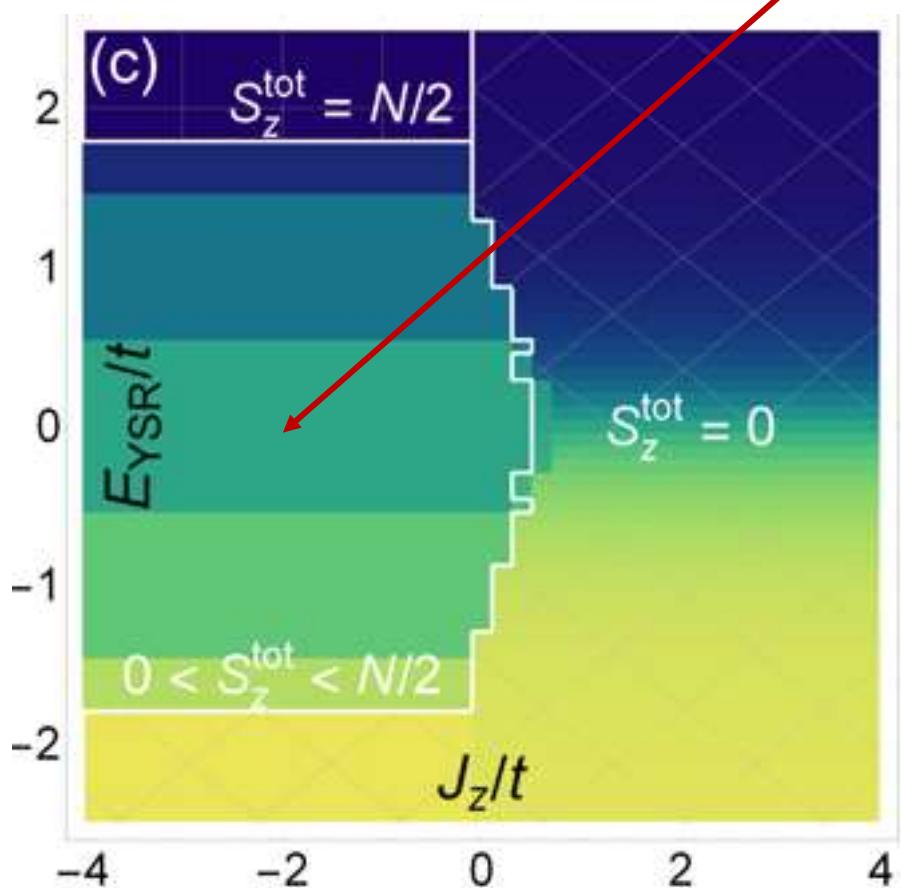
Mapping to t-J model (spin 1/2)



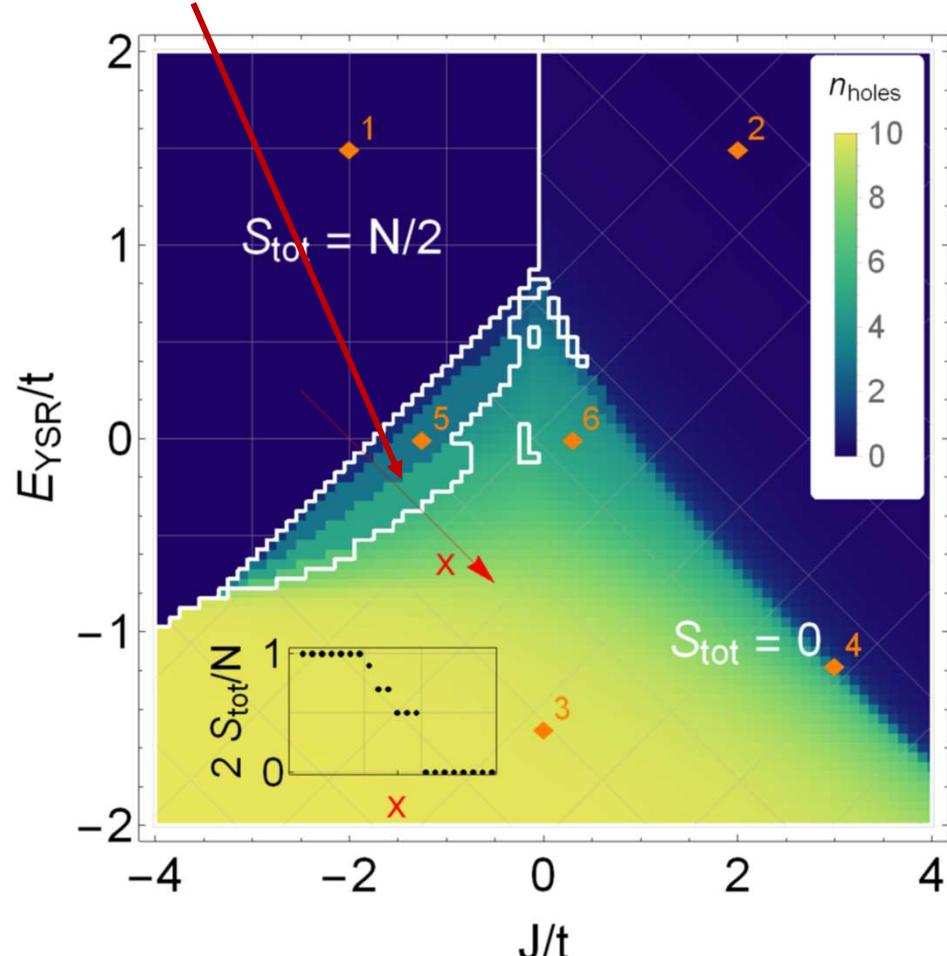
$$H = \sum_j \left\{ -E_{\text{YSR}} n_j + J \mathbf{S}_j \cdot \mathbf{S}_{j+1} - \tilde{t} \sum_{\sigma} [d_{j,\sigma}^{\dagger} d_{j+1,\sigma} + \text{h. c.}] + \tilde{\Delta} [d_{j,\downarrow}^{\dagger} d_{j+1,\uparrow}^{\dagger} - d_{j,\downarrow} d_{j+1,\uparrow} + \text{h. c.}] \right\}$$

Phase diagram ($S=1/2$)

Parent state for top. SC



classical

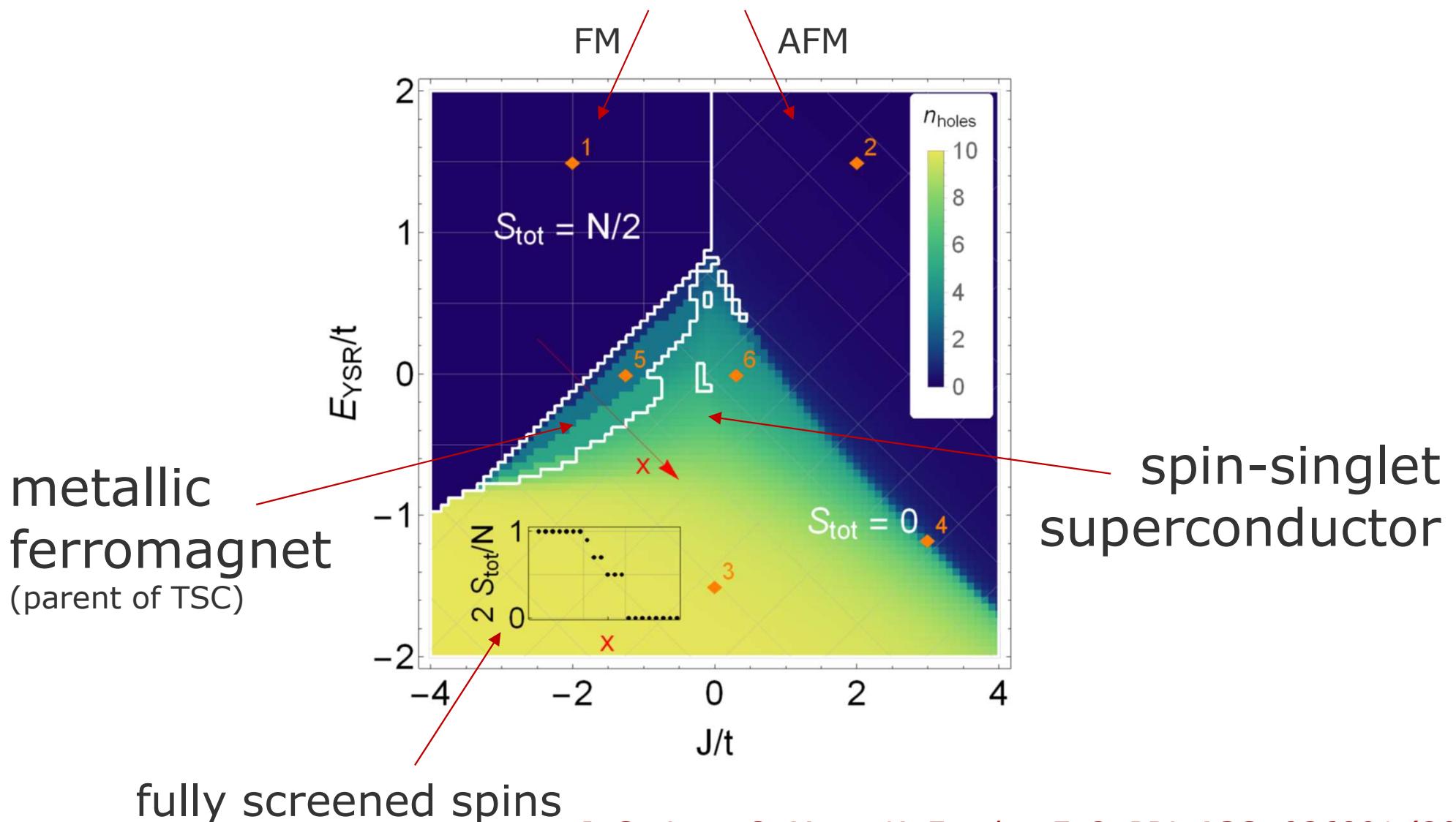


quantum

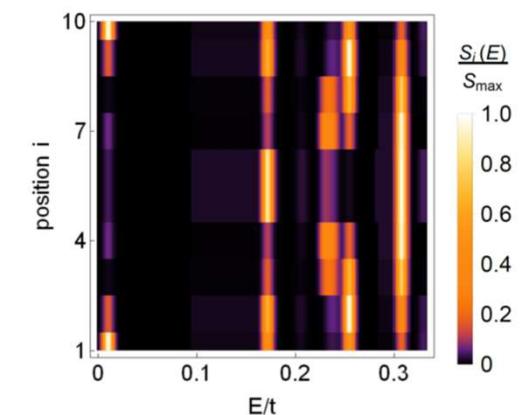
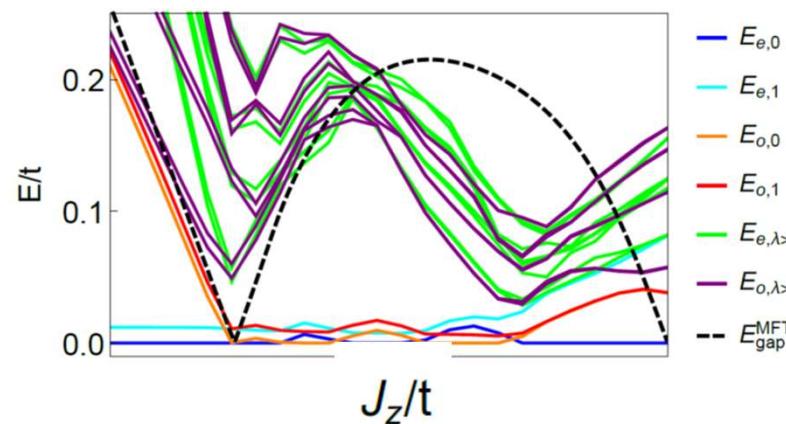
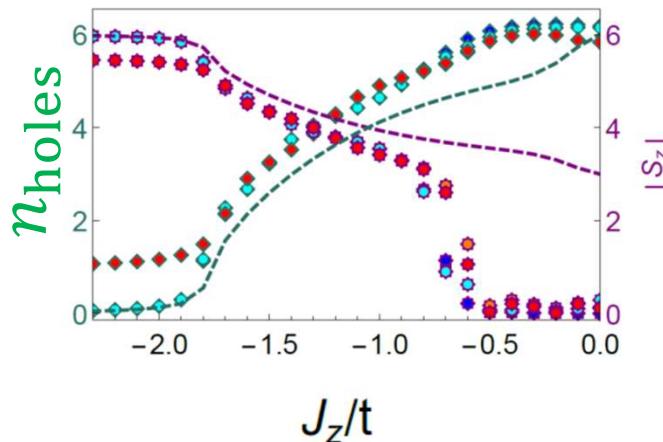
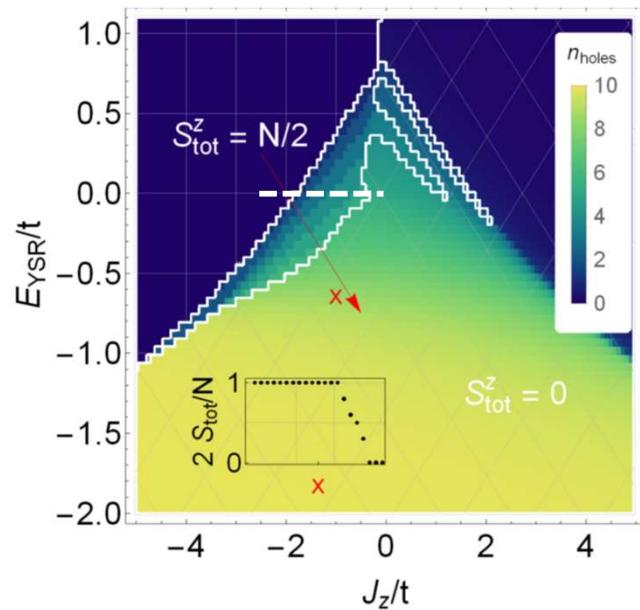
J. Steiner, C. Mora, K. Franke, FvO, PRL 128, 036801 (2022)

Phase diagram

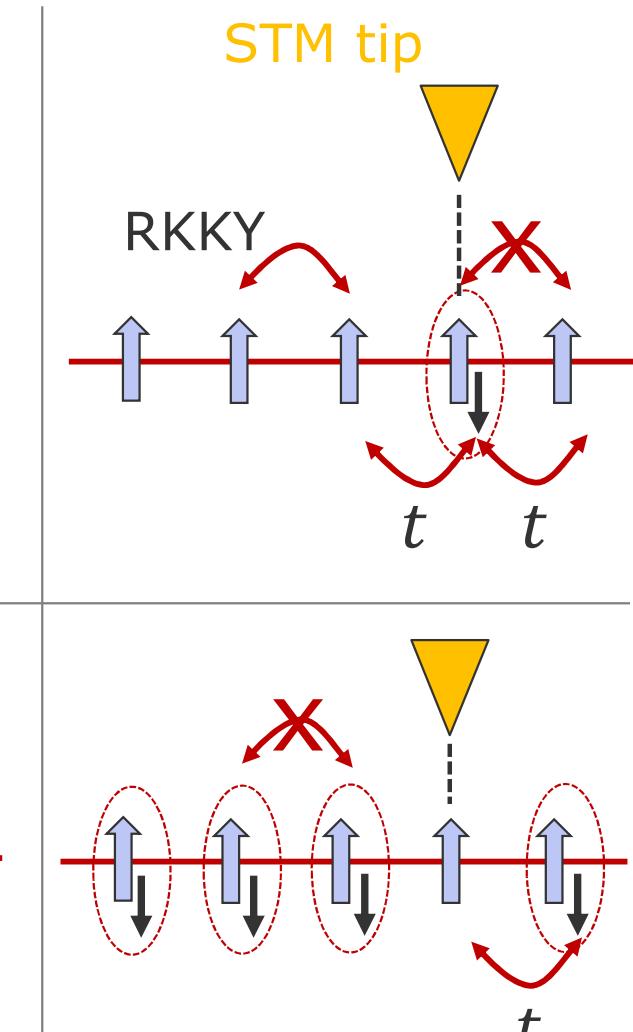
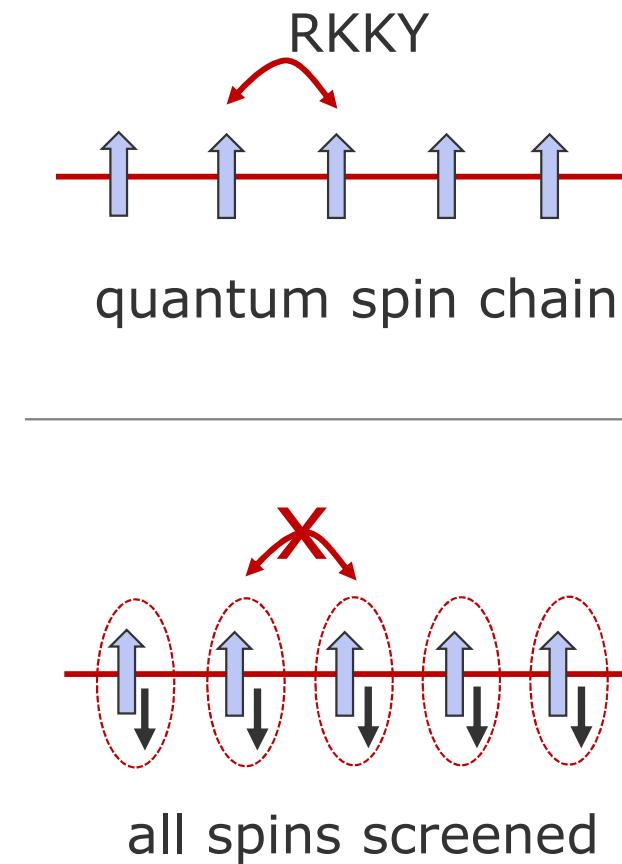
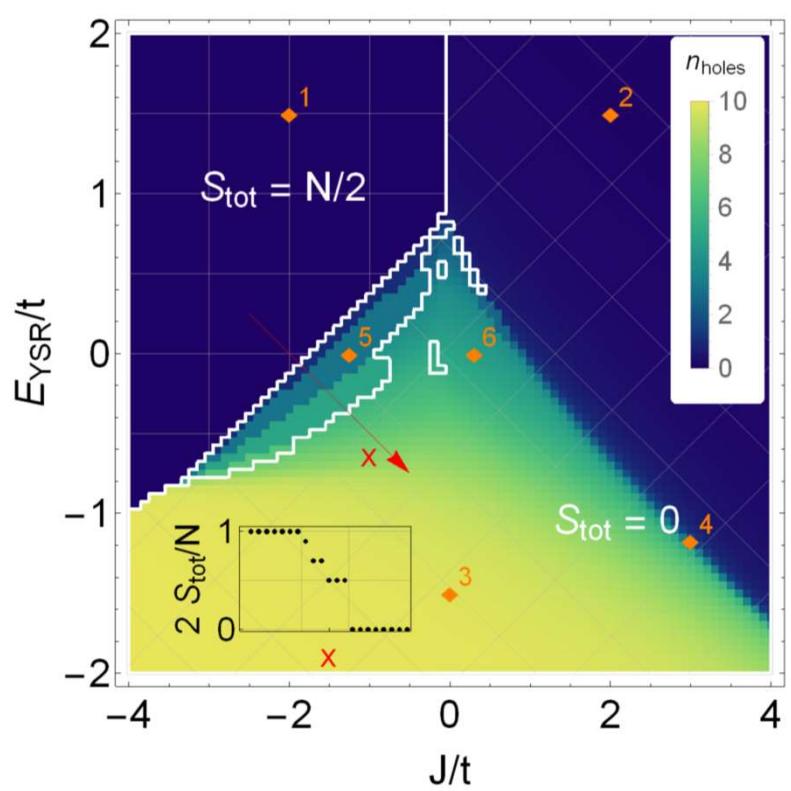
spin-1/2 Heisenberg chain



Metallic ferromagnet & topological superconductivity



Local excitation spectra



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Conclusions

- YSR states in real metals: Importance of higher spins, multiple channels, single-ion anisotropy
 - Zero-bandwidth model: Qualitatively reproduces NRG calculations
 - Quantum spins: screened adatom spin & Kramers degeneracy
 - Chains: Mapping to t-J model & reduced phase space for TSC
 - Diode behavior in JJs with single magnetic atom
-
- *Yu-Shiba-Rusinov states in real metals*
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 - *Quantum magnetism and topological superconductivity in Yu-Shiba-Rusinov chains*
J. Steiner, C. Mora, K. Franke, FvO, PRL **128**, 036801 (2022)
 - *Quantum Yu-Shiba-Rusinov dimers*
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 - *Quantum spins and hybridization in magnetic chains on a SC*
Liebhaber, ..., FvO, K. Franke, Nature Comm. **13**, 2160 (2022)
 - *Diode behavior in JJs w/ magnetic atom*
M. Trahms, L. Melischek, J. Steiner..., FvO, K. Franke, submitted

