TT 66: Superconductivity: Yu-Shiba-Rusinov and Andreev Physics

Time: Thursday 9:30–12:30 Location: H 3005

TT 66.1 Thu 9:30 H 3005

Proximity-superconductivity of noble metal surface states — •Christian von Bredow, Lucas Schneider, Howon Kim, Torben Hänke, Khai That Ton, Kirsten von Bergmann, Jens Wiebe, and Roland Wiesendanger — Department of Physics, University of Hamburg, Hamburg, Germany

Adding superconductivity to gapless materials via the proximity effect can lead to a variety of interesting physical phenomena including topologically non-trivial states [1,2,3]. Rashba-split surface states, proximitized by a superconducting substrate, have recently been of particular interest as they combine large spin-orbit coupling with a large superconducting gap, making them a popular system in the search for topological superconductivity [4].

We study the mechanism of proximity-induced superconductivity in the Shockley-type surface states of thin films of Cu and Ag, grown on Nb(110), the elemental superconductor with the highest critical temperature, via STM. The tunneling spectra exhibit a multitude of sharp peaks at low energies, which can be assigned to two types of Andreev-bound states in the thin film and in the surface state.

[1] L. Schneider et al., Nature 621 (2023) 60
[2] J. Ortuzar et al., Phys. Rev. B 108 (2023) 024511
[3] T. Tomanic et al., Phys. Rev. B 94 (2016) 220503(R)
[4] A. C. Potter et al., Phys. Rev. B 85 (2012) 094516

TT 66.2 Thu 9:45 H 3005

Observation of zero-energy modes in Gd atomic chains on superconducting Nb(110) — •Yu Wang — Physikalisches Institut, Experimentelle Physik II, Universitaet Wuerzburg, Am Hubland, D-97074 Würzburg, Germany

The proposal to generate topologically protected edge states by linking Yu-Shiba-Rusinov states within a 1D chain of magnetic adsorbates has sparked considerable interest to the study of YSR states. Numerous research studies have been conducted on 3d transition metals placed on various superconducting substrates. In contrast, experimental results for 4f -shell rare-earth metals are scarce. However, rare-earth metals such as Gd, Tb, Dy, on superconductors are highly intriguing owing to highly localized strong magnetic moment of the 4f orbital which is primarily screened by outer electronic shells. In this experimental study, we investigate Yu-Shiba-Rusinov states induced by Gd adatoms on a superconducting Nb(110) surface. We are able to engineer Gd atom chains along the substrate's [110] and [001] directions, revealing distinct behaviors in differently oriented chains. [110]-oriented Gd chains exhibit spectroscopic features at their ends, identifying them as trivial edge states, while [001]-oriented Gd chains display zero-energy edge states, suggesting non-trivial nature.

TT 66.3 Thu 10:00 H 3005

First principles analysis of Gd nanostructures on superconducting Nb(110) — •David Antognini Silva[1], Philipp Rüssmann[1,2], and Stefan Blügel[1] — [1]Peter Günberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [2]Würzburg University, Germany

Materials that combine magnetism, spin-orbit interaction and conventional *s*-wave superconductivity are a suitable platform to study Yu-Shiba-Rusinov (YSR) states [1-3] and Majorana zero modes (MZM) [4], that can be used as building blocks of fault-tolerant topological qubits.

Recently, STM experiments for Gd chains on Nb(110) surface showed indication of MZMs at the ends of the chains [5]. To better understand the nature of those modes, we implemented the Bogoliubov-de Gennes (BdG) formalism in the juKKR impurity code [6] that allows the material-specific description of defects in superconductors from first principles, and applied it to Gd adatom nanostructures placed on the superconducting Nb(110) surface. We analyze the YSR states arising from the coupling of the magnetic Gd atoms and investigate their dependence on the geometry of the nanocluster and its magnetic ordering.

This work was funded by the DFG through Germany's Excellence Cluster ML4Q (EXC 2004/1 - 390534769).

[1] L. Yu, Acta Physica Sinica **21** (1965) 75
[2] H. Shiba, Prog. Theor. Phys. **40** (1968) 435
[3] A. I. Rusinov, Sov. J. Exp. Theor. Phys. **29** (1969) 1101
[4] Nadj-Perge *et al.*, Science **346** (2014) 6209
[5] Y. Wang *et al.*, arXiv.2311.09742
[6] https://iffgit.fz-juelich.de/kkr/jukkr

TT 66.4 Thu 10:15 H 3005

Andreev reflection in single-molecule junctions — •Lorenz Meyer, Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

Electron transport across a single phthalocyanine (2H-Pc) molecule on Pb(111) is explored with a scanning tunneling microscope. The two variants of the molecule, 2H-Pc and pyrrolic-H abstracted Pc, behave differently when a normal-metal tip is vertically approached. While 2H-Pc shows a gradually increasing zero-bias resonance in spectra of the differential conductance with decreasing tip-molecule separation, spectroscopy of Pc reveals an invariant Bardeen-Cooper-Schrieffer energy gap. These results are discussed in terms of Andreev reflection and the occurrence of Yu-Shiba-Rusinov bound states.

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TT 66.5 Thu 10:30 H 3005

Ab-initio investigation of Yu-Shiba-Rusinov states of 3*d* adatoms interacting with Rashba-split surface states — •Ilias Klepetsanis[1,2], Philipp Rüssmann[1,3], Jens Wiebe[4], and Samir Lounis[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany — [3]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [4]Universität Hamburg, 20355 Hamburg, Germany

The interplay between magnetism and superconductivity has long been under the scope of condensed matter physics research, as two seemingly competing phenomena of order. Here, we employ the Bogoliubov-de-Gennes full-potential relativistic Korringa-Kohn-Rostoker Green function method [1] to study Yu-Shiba-Rusinov states emerging when 3*d* magnetic adatoms are interfaced with different spacers deposited on Nb surfaces. These spacers are heavily investigated to introduce Rashba surface states and engineer the strength of spin-orbit coupling at the vicinity of a superconductor, which leads to unconventional superconducting pairing [2]. In particular, we explored the cases of (111) films of Cu, Ag, Au as well as $BiAg_2$/Ag and $BiCu_2$/Cu.

We acknowledge funding by the DFG (SPP 2244; LO 1659/7-1; ML4Q Cluster of Excellence EXC 2004/1 – 390534769).

[1] P. Rüßmann, S. Blügel, Phys. Rev. B **105** (2022) 125143
[2] P. Rüßmann *et al.*, Phys. Rev. Research **5** (2023) 043181

TT 66.6 Thu 10:45 H 3005

Full counting statistics of Yu-Shiba-Rusinov bound states — •David Christian Ohnmacht[1], Wolfgang Belzig[1], and Juan Carlos Cuevas[2] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

We adapt the concept of full counting statistics (FCS) to provide the deepest insight thus far into the spin-dependent transport in systems containing Yu-Shiba-Rusinov (YSR) states [1]. Such systems include single-impurity junctions with a normal and a superconducting (SC) STM tip, as well as double-impurity systems [2]. The FCS concept allows us to identify every tunneling process that plays a role in these situations and to classify them according to the charge transferred in them. In particular, our approach is able to reproduce the experimental results recently reported on the shot noise of a single-impurity junction with a normal STM tip [3]. We also predict the signatures of resonant multiple Andreev reflections in the shot noise of single-impurity junctions with two SC electrodes and show that the FCS approach allows us to understand conductance features that have been incorrectly interpreted in the literature. In the case of double-impurity junctions we show that the direct tunneling between YSR states is characterized by a strong reduction of the Fano factor that reaches a minimum value of 7/32.

[1] D. C. Ohnmacht et. al., Phys. Rev. Res. 5 (2023) 033176
[2] H. Huang et. al., Nat. Phys. 16 (2020) 1227

[3] U. Thupakula et. al., Phys. Rev. Lett. 128 (2022) 247001

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TT 66.7 Thu 11:15 H 3005

DC Josephson effect between two Yu-Shiba-Rusinov bound states — •Wolfgang Belzig[1], Subrata Chakraborty[1], Danilo Nikolic[2], Ruben Suano Souto[3], and Juan Carlos Cuevas[3] — [1]Universität Konstanz — [2]Universität Greifswald — [3]UA MAdrid

Motivated by recent experiments [1], we present here a theoretical study of the DC Josephson effect in a system comprising two magnetic impurities coupled to their respective superconducting electrodes and which exhibit Yu-Shiba-Rusinov (YSR) states. Using a mean-field Anderson model with broken spin symmetry to compute the supercurrent in this system for an arbitrary range of parameters (coupling between the impurities, orientation of the impurity spins, etc.). We predict a variety of physical phenomena such as (i) the occurrence of multiple 0-π transitions in the regime of weak coupling that can be induced by changing the energy of the YSR states or the temperature; (ii) the critical current strongly depends on the relative orientation of the impurity spins and it is maximized when the spins are either parallel or antiparallel, depending on the ground state of the impurities; and (iii) upon increasing the coupling between impurities, triplet superconductivity is generated in the system and it is manifested in a highly nonsinusoidal current-phase relation. Our predictions can be tested experimentally with the existing realization of this system and the main lessons of this work are of great relevance for the field of superconducting spintronics.

[1] Nat. Phys. 16 (2020) 1227
[2] S. Chakraborty, D. Nikolić, R. S. Souto, W. Belzig, J. C. Cuevas, Phys. Rev. B 108 (2023) 094518

TT 66.8 Thu 11:30 H 3005

Identifying Ising superconductors - The role of unconventional Andreev reflection in the formation of bound states — •Michael Hein[1], Juan Carlos Cuevas[2], and Wolfgang Belzig[1] — [1]Universität Konstanz — [2]Universidad Autónoma de Madrid

Magnetic impurities on superconducting surfaces induce so called *Yu-Shiba-Rusinov* (YSR) bound states. They have been widely studied using scanning tunnelling microscopy (STM) with substrates made of conventional superconductors [1]. In this work we investigate theoretically whether and how these states occur in unconventional Ising superconductors [2]. One of our main findings is the existence of subgap states even in the case of non-magnetic impurities. To shed light on the origin of these states, we also study the unconventional Andreev reflection at the interface between an Ising superconductor and a normal metal. This work paves the way for the understanding of the proximity effect in Ising superconductors and predicts different transport signatures that would allow to experimentally identify Ising superconductors.

[1] B. W. Heinrich et al., Prog. Surf. Sci. 93 (2018) 1
[2] G. Tang et al., Phys. Rev. Lett. 126 (2021) 237001

TT 66.9 Thu 11:45 H 3005

Thermocurrent spectroscopy of Yu-Shiba-Rusinov states in single-molecule junctions — •Pascal Gehring — IMCN/NAPS, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

The interaction between magnetic impurities and superconductors leads to fascinating phenomena resulting from the competition between Kondo screening and Cooper pair formation. For example, individual magnetic impurities can form states within the superconducting gap, called Yu-Shiba-Rusinov (YSR) bound states, that create sharp features in the density of states. Here, We employ our recently developed thermocurrent spectroscopy set-up to experimentally study the thermoelectric properties of a neutral and stable all-organic radical molecule coupled to proximity induced superconducting break-junction electrodes at millikelvin temperatures. We find that the sharp YSR features also result in a strong enhancement of their thermoelectric response. By varying the external magnetic field a quantum phase transition from the Kondo into the YSR regime is induced with a twofold increase of the thermoelectric current.

TT 66.10 Thu 12:00 H 3005

Impact of evanescent scattering modes in short junctions — •Daniel Kruti and Roman-Pascal Riwar — Jülich Research Centre and Cologne University

Superconducting junctions are essential building blocks for quantum hardware, and their fundamental behaviour is still a highly active research field. For generic junctions, the emergence of subgap Andreev bound states is conveniently described by Beenakker's formula, representing an important starting point for both analytic and numeric studies. In this work, we critically reassess two common assumptions: that in the short junction limit scattering is approximately energy independent and dominated by planar channels. We argue that cross-channel scattering can lead to a strong energy-dependence which is particularly pronounced when the system is tuned close to a change of the channel number – even if energy is small compared to the Thouless energy. We provide a general recipe to include evanescent modes, and apply it to the example of a ballistic junction with nontrivial geometry. We show that the interplay between evanescent modes and energy-dependant scattering has a significant influence on the Andreev spectrum, especially close to the superconducting gap. In particular, the energy-dependence of the scattering matrix breaks the symmetry which allows for the Andreev spectrum to touch the gap. Evanescent modes effectively restore this symmetry. We expect our work to be relevant for contemporary experimental and theoretical studies of ultra-small junctions and their (dissipative) transport properties.

TT 66.11 Thu 12:15 H 3005

On-demand population of Andreev levels by their ionization in the presence of Coulomb blockade — •Aleksandr Svetogorov[1], Wolfgang Belzig[1], Pavel Kurilovich[2], Vladislav Kurilovich[2], Michel Devoret[2], and Leonid Glazman[2] — [1]Universität Konstanz, Konstanz, Germany — [2]Yale University, New Haven, USA

A mechanism to deterministically prepare a nanowire Josephson junction in an odd parity state is proposed. The mechanism involves population of two Andreev levels by a resonant microwave drive breaking a Cooper pair, and a subsequent ionization of one of the levels by the same drive. Robust preparation of the odd state is allowed by a residual Coulomb repulsion in the junction. A similar resonant process can also be used to prepare the junction in the even state. Our theory explains a recent experiment [1].

[1] J. J. Wesdorp et al., Phys. Rev. Lett. 131 (2023) 117001