TT 8: Yu-Shiba-Rusinov Systems

Time: Monday 15:00–17:15 Location: HSZ 103

Invited Talk TT 8.1 Mon 15:00 HSZ 103

Molecules on a superconductor: Inducing magnetism and resonance-enhanced vibrational spectroscopy — •Richard Berndt[1], Jan Homberg[1], Alexander Weismann[1], Manuel Gruber[2], and Troels Markussen[3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, Germany — [3]Synopsys Denmark, Copenhagen, Denmark

Magnetic impurities can induce so-called Yu-Shiba-Rusinov (YSR) resonances in the energy gap of a superconductor. We use these resonances for spin detection in a scanning tunneling microscope and demonstrate that diamagnetic phthalocyanine molecules acquire a spin when they are arranged into supramolecular arrays on superconducting Pb(100). Spectroscopy and modeling reveal that the electrostatic fields of its neighbors render a molecule paramagnetic.

Inelastic tunneling spectroscopy of vibrational excitations usually suffers from low sensitivity and limited spectral resolution. We harness YSR resonances to enhance the inelastic signal by more than an order of magnitude and to improve the energy resolution beyond the thermal broadening limit. As a result, 46 vibrational peaks are resolved from Pb-phthalocyanine enabling a comparison with calculated modes. The method may help to further probe the interaction of molecules with their environment and to better understand selection rules for vibrational excitations.

TT 8.2 Mon 15:30 HSZ 103

Yu-Shiba-Rusinov impurity bound states in superconductors from first principles — •David Antognini Silva[1], Philipp Rüssmann[1,2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]Würzburg Universität, Germany

Materials that combine magnetism, spin-orbit interaction and conventional s-wave superconductivity are a suitable platform to study Majorana zero modes (MZM) [1], that can be used as building blocks of fault-tolerant topological qubits. In general, magnetic impurities in superconductors leads to localized Yu-Shiba-Rusinov (YSR) states at the impurity [2]. Understanding their interplay with MZMs is crucial to achieve topological quantum computers in the future.

In our work, we implemented the Bogoliubov-de Gennes (BdG) formalism in the juKKR Korringa-Kohn-Rostoker Green function impurity code (https://iffgit.fz-juelich.de/kkr/jukkr) to allow the material-specific description of defects perfectly embedded in superconductors from first principles. We apply it to an Fe impurity embedded in bulk Pb in the normal and superconducting state, then analyse the YSR states of different magnetic transition-metal adatoms placed on a superconducting Nb(110) surface where the influence of the impurity-substrate distance on the energy of the YSR states is discussed.

[1] Nadj-Perge *et al.*, Science **346**, 6209 (2014)
[2] L. Yu, Acta Physica Sinica **21**, 75 (1965)
H. Shiba, Prog. Theor. Phys. **40**, 435 (1968) A. I. Rusinov, Sov. J. Exp. Theor. Phys. **29**, 1101 (1969)

TT 8.3 Mon 15:45 HSZ 103

Yu-Shiba-Rusinov states of quantum impurities in spin-split superconductors — •Anastasiia Skurativska[1], Jon Ortuzar[2], Sebastian Bergeret[1,3], Dario Bercioux[1,4], and Miguel Angel Cazalilla[1,4] — [1]DIPC, 20018 San Sebastian, Spain — [2]CIC nanoGUNE-BRTA, 20018 San Sebastian, Spain — [3]CFM-MPC Centro Mixto CSIC-UPV/EHU, 20018 San Sebastian, Spain — [4]IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain

Yu-Shiba-Rusinov (YSR) states arise as a sub-gap excitations in a system of magnetic impurity coupled to a superconducting host. Despite the quantum nature of their spin degree of freedom, magnetic impurities in such systems are often described by a classical spin. Taking into account quantum nature of the impurity-spin has proven to give useful insights into the ground-state and excitation properties of the magnetic impurity-superconductor system.

Here, we report on the spectral properties of the YSR states of a magnetic impurity on a spin-split superconductor. Using the zero-bandwidth approximation we obtain the spectral function of the YSR states. Unlike the classical model which predicts full spin polarization for the YSR peaks, we find the quantum model predicts partial polarization. The parity-changing phase transition switches the spin polarization of the YSR peaks after crossing at the center of the superconducting gap. We discuss the possibility of using this effect as a tunable spin-filter in a quantum dot or a molecule in proximity to a spin-split superconductor.

TT 8.4 Mon 16:00 HSZ 103

Building crystalline topological superconductors from Shiba lattices — •Martina Ondina Soldini[1], Felix Küster[2], Glenn Wagner[1], Souvik Das[2], Amal Aldarawsheh[3,5], Ronny Thomale[4,6], Samir Lounis[3,5], Stuart S. P. Parkin[2], Paolo Sessi[2], and Titus Neupert[1] — [1]University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Jülich, Germany — [4]Institut fur Theoretische Physik und Astrophysik, Universitat Wurzburg, Wurzburg, Germany — [5]Faculty of Physics, University of Duisburg-Essen and CENIDE, Duisburg, Germany — [6]Department of Physics and Quantum Centers in Diamond and Emerging Materials (QuCenDiEM) Group, Indian Institute of Technology Madras, Chennai, India

Majorana boundary modes are the key feature of topological superconductors. Lattices of Shiba bound states, arising from magnetic adatoms placed on the surface of a conventional superconductor, may host these topological excitations. With scanning tunneling microscopy we create and probe adatom lattices to create topological crystalline superconductors. We combine theoretical modeling and experimental analysis to reveal signatures consistent with mirror-symmetry protected topological superconductors, hosting edge and higher-order corner states. Our results show the immense versatility of Shiba lattices to design the topology of 2D superconductors.

TT 8.5 Mon 16:15 HSZ 103

Mn clusters on superconducting Ta(110) surface — •András Lászlóffy[1], Bendegúz Nyári[2,3], László Szunyogh[2], and Balázs Újfalussy[1] — [1]Wigner Research Centre for Physics, Budapest, Hungary — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]ELKH-BME Condensed Matter Physics Research Group, Hungary

Over the past decade, the formation of Yu-Shiba-Rusinov (YSR) states around magnetic impurities proximity coupled to superconducting materials raised considerable interest. The hybridization between these states leads to bands in magnetic chains being potential candidates for hosting Majorana edge states. In this work we solve the Bogoliubov-de Gennes equation as implemented in the first-principles Korringa-Kohn-Rostoker Green's function method. First, we provide an in-depth analysis of the YSR states of a single Mn adatom on Ta(110), and the hybridization between them in Mn dimers. We then study the formation of a minigap and zero energy states in chains with various directions and nearest-neighbor distances, making a strong implication that Majorana zero modes can emerge in these systems.

TT 8.6 Mon 16:30 HSZ 103

Effect of Fe impurities on the superconducting state of Ir/Nb overlayer — •Bendegúz Nyári[1,2], András Lászlóffy[3], Krisztián Palotás[3], László Szunyogh[1,2], Levente Rózsa[4], and Balázs Újfalussy[3] — [1]Department of Theoretical Physics, Budapest University of Technology and Economics, Hungary — [2]ELKH-BME Condensed Matter Physics Research Group, Hungary — [3]Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, Hungary — [4]Department of Physics, University of Konstanz, Germany

Artificial magnetic chains on top of superconducting surfaces, where in the presence of large spin-orbit coupling or non-collinear magnetic states a topological gap can appear, are potential candidates to host Majorana edge states. Iridium as an overlayer on various metallic substrates appeared to be a good platform for the formation of spin-spiral states in magnetic overlayers and chains.

By solving the relativistic Bogoliubov–de Gennes equations, first we investigate the superconducting properties of 10 monolayers of Ir on top of Nb(110) surface. In the Ir layer we observe a strong reduction of the superconducting order parameter, but the gap just slightly decreases as compared to bulk Nb. Then the effect of Fe impurities on the

superconducting state is studied in different setups. For a single Fe impurity we find a huge spatial extension of the Yu–Shiba–Rusinov states. Disordered Fe impurities modelled within the coherent-potential approximation in the dilute concentration limit seem to rapidly destroy the superconducting state of the Ir overlayer.

TT 8.7 Mon 16:45 HSZ 103

Yu-Shiba-Rusinov states in small Fe clusters on Pb(111) — •Nora Kucska, Krisztián Palotás, Andras Laszloffy, and Balazs Ujfalussy — Wigner Research Centre for Physics, Budapest, Hungary

By solving the fully relativistic Bogoliubov-de Gennes equations by band-theoretical methods, we investigate the Yu-Shiba-Rusinov (YSR) states of single, double and triple magnetic Fe adatoms on the top of Pb(111) surface. First, we show that the local density of states in the normal state plays a key role in the formation of the YSR states that appear in the interior of the superconducting gap. We discuss the effects of different atomic arrangements, the role of lattice relaxations and various spin configurations on the YSR states, and we compare our results to recent experiments.

TT 8.8 Mon 17:00 HSZ 103

Yu-Shiba-Rusinov band dispersion of an infinite chain on a semi-infinite surface — •Rik Broekhoven, Artem Pulkin, Antonio Manesco, Sander Otte, Anton Ahkmerov, and Michael Wimmer — Delft University of Technology, Delft, the Netherlands

Chains of magnetic atoms on s-wave superconductors have been proposed to become topological superconductors, when their in-gap Yu-Shiba-Rusinov (YSR) band is p-wave gapped by for example spin-orbit coupling. As recently shown through STM experiment, however, realistic systems have many YSR bands and relatively small spin-orbit coupling limiting the topological phase. Ab initio models can help to increase our understanding and find regions of material and parameter space where the system is still predicted to be topological. These finite-size simulations must however overestimate the superconducting gap to ensure the system is smaller than the superconductor coherence length.

We combine ab initio calculation with multi-dimensional Green's functions formalism to extend the model beyond this limit. This allows us to do calculations with realistic gap size. We compute the dispersion of an infinite chain on top of a semi-infinite surface. We focus on Mn atoms on Nb(110) and show how our model compares with the dispersion measured by Schneider et al. in 2021.