SFB 1432

Special Seminar

Universität Konstanz

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Talk at 15:15
in P 603
refreshment afterwards

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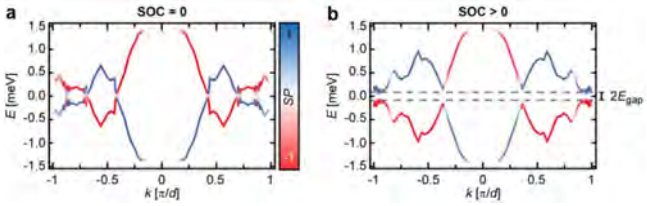
Influence of the Spin Configuration on the Band Structure of Yu-Shiba-Rusinov States



Magnetic impurities in conventional superconductors locally break Cooper pairs, leading to the emergence of Yu-Shiba-Rusinov (YSR) bound states. Chains of YSR impurities have been theoretically predicted to give rise to Majorana bound states, which are promising for the realization of topological quantum computers. A fundamental understanding of the formation of YSR states in small atomic clusters is essential for revealing the topological properties of the YSR band structure. The accurate theoretical modelling of YSR states represents a considerable challenge, since it requires a simultaneous description of the electronic structure, the magnetic ordering of the impurities and superconductivity on significantly different energy scales.
Here, first-principles simulations are combined with tight-binding model calculations to determine the influence of the electronic and magnetic properties on the band structure of YSR states. In ferromagnetic chains the spin-orbit coupling opens a minigap in the bands around the Fermi energy where end states are formed, but the small size of this gap in typical material platforms is found to lead to a long-range extension and interactions between these precursors of Majorana bound states [1]. Introducing nonmagnetic heavy-metal capping layers proximity coupled to the superconductor is expected to enhance the spin-orbit coupling, yet it may fail to considerably increase the size of the minigap in ferromagnetic chains [2]. The minigap is larger in antiferromagnetic chains where the spin-orbit coupling is not necessary for its formation, but the well-localized end states in this minigap typically have a topologically trivial origin [3]. The theoretical concepts are illustrated by experimental realizations in specific materials.

[1] L. Schneider, P. Beck, J. Neuhaus-Steinmetz, L. Rózsa, T. Posske, J. Wiebe, and R. Wiesendanger, Nat. Nanotechnol. 17, 384 (2022).
[2] P. Beck, B. Nyári, L. Schneider, L. Rózsa, A. Lászlóffy, K. Palotás, L. Szunyogh, B. Ujfalussy, J. Wiebe, and R. Wiesendanger, Commun. Phys. 6, 83 (2023).
[3] L. Schneider, P. Beck, L. Rózsa, T. Posske, J. Wiebe, and R. Wiesendanger, Nat. Commun. 14, 2742 (2023).

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