TT 36: Superconductivity: Theory I

Time: Wednesday 9:30–13:00 Location: H 3005

TT 36.1 Wed 9:30 H 3005

Interorbital Cooper pairing at finite energies in Rashba surface states — •Philipp Rüssmann[1,2], Masoud Bahari[1], Stefan Blügel[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany

Multiband effects in hybrid structures provide a rich playground for unconventional superconductivity. We combine two complementary approaches based on density-functional theory (DFT) [1] and effective low-energy model theory in order to investigate the proximity effect in a Rashba surface state in contact with an s-wave superconductor [2]. We discuss these synergistic approaches and combine the effective model and DFT analysis at the example of a Au/Al heterostructure. This allows us to predict finite-energy superconducting pairing due to the interplay of the Rashba surface state of Au, and hybridization with the electronic structure of superconducting Al. We investigate the nature of the induced superconducting pairing, and we quantify its mixed singlet-triplet character. Our findings demonstrate general recipes to explore real material systems that exhibit interorbital pairing away from the Fermi energy.

This work was supported by the Bavarian Ministry of Economic Affairs, Regional Development and Energy and the ML4Q Cluster of Excellence (EXC 2004/1 - 390534769).

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

TT 36.2 Wed 9:45 H 3005

Beyond the Fermi surface: full-bandwidth Migdal-Eliashberg superconductivity in superhydrides — •Roman Lucrezi[1], P. P. Ferreira[1,2], S. Hajinazar[3], H. Mori[3], H. Paudyal[3], E. R. Margine[3], and C. Heil[1] — [1]Graz Univ. of Techn. Austria — [2]Univ. de São Paulo, Brazil — [3]Binghamton Univ., USA

We present an ab-initio implementation of the full-bandwidth anisotropic Migdal-Eliashberg theory to overcome the shortcomings of the constant-DOS approach in describing superconducting properties in materials with narrow bands or critical points near the Fermi level. In contrary to the constant-DOS approach, the full-bandwidth theory takes into account electron scattering processes beyond the Fermi surface within a self-consistent determination of the mass renormalization function, energy shift, and order parameter at various temperatures while maintaining charge neutrality. We demonstrate the effectiveness of our implementation by applying it to two classes of near room-temperature superhydrides: the sodalite-like clathrates YH_6 and CaH_6, as well as the covalently-bonded H_3S and D_3S. In addition, we investigate the effects of maximizing the density of states at the Fermi level for topical electron- and hole-doped superhydrides. We compare the new full-bandwidth treatment to the previous constant-DOS approximation and reveal significant improvements in describing the superconducting state with our advanced implementation. This not only enhances precision but also offers computational efficiency, and thus provides new perspectives on high-accuracy predictions in superconductivity research.

TT 36.3 Wed 10:00 H 3005

Stability of Bogoliubov Fermi Surfaces within BCS Theory — Ankita Bhattacharya[1,2] and •Carsten Timm[2] — [1]Department of Physics and Astronomy, Uppsala University, Box 516, 75120 Uppsala, Sweden — [2]Institute of Theoretical Physics, TU Dresden, 01062 Dresden, Germany

It has recently been realized that the gap nodes of multiband superconductors that break time-reversal symmetry generically take the form of Fermi surfaces of Bogoliubov quasiparticles. These Fermi surfaces lead to a nonzero density of states (DOS) at the Fermi energy, which typically disfavors such superconducting states. It has thus not been clear whether these states can be stable for reasonable pairing interactions or are preempted by time-reversal-symmetric states with vanishing DOS. Applying BCS theory to a paradigmatic model, we show that the time-reversal-symmetry-breaking states are indeed stabilized over broad parameter ranges at weak coupling [1]. Moreover, we introduce a fast method that involves solving the inverse BCS gap equation, does not require iteration, does not suffer from convergence problems, and can handle metastable solutions.

[1] A. Bhattacharya, C. Timm, Phys. Rev. B **107** (2023) L220501

TT 36.4 Wed 10:15 H 3005

Bogoliubov-Fermi Surfaces in 2D heterostructures — •Julia Link and Carsten Timm — TU Dresden, Germany

A characteristic feature of the superconducting state in BCS theory is the appearance of a full gap in the quasiparticle spectrum. Under various conditions, one can instead obtain an exotic form of superconductivity for which the superconducting gap contains Bogoliubov Fermi surfaces (BFSs). A BFS is a $d-1$-dimensional surface of zero-energy states in the d-dimensional momentum space. BFSs were recently observed in the two-dimensional heterostructure Al-InAs in an applied in-plane magnetic field [1]. In this talk, we present the theoretical prediction for the density of states of such a system and predict the temperature dependence of observables such as the heat capacity and the superfluid density in the presence of BFSs.

[1] Phan et al., Phys. Rev. Lett. **128** (2022) 10770

TT 36.5 Wed 10:30 H 3005

Thermoelectric Switch From Bogoliubov Fermi Surface in superconducting 3D Topological Insulator Heterostructures — •Phillip Mercebach[1], Bo Lu[2], Keiji Yada[3], Yukio Tanaka[3], and Pablo Burset[1] — [1]Department of Theoretical Condensed Matter Physics, Condensed Matter Physics Center (IFIMAC) and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [2]Department of Physics, Tianjin University, Tianjin 300072, China — [3]Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan

A weak magnetic field applied to a superconductor (SC) can selectively close the superconducting gap, giving rise to a segmented Fermi surface. So-called Bogoliubov Fermi surfaces (BFSs) have been observed in recent experiments in a three-dimensional topological insulator (3DTI) in proximity to a SC. Here, we employ a scattering matrix formalism to reveal signatures of the BFS in the thermoelectric transport properties of a superconducting hybrid junction on the surface of a 3DTI. We consider a setup with two normal probes (N) connected to a SC (N-SC-N configuration) to study local and nonlocal transport under an applied in-plane magnetic field. With a temperature gradient, the magnetic field creates equal local and nonlocal electric Seebeck currents which follow the orientation of the BFS. Furthermore, we predict a switch in the required voltage bias enabling local and nonlocal Peltier cooling, which again depends on the orientation of the BFS. As a result, our work opens new perspectives for applications in spintronics and exploring unconventional superconducting phases.

TT 36.6 Wed 10:45 H 3005

Complete zero-energy flat bands of surface states in fully gapped chiral noncentrosymmetric superconductors — •Clara Johanna Lapp[1,2], Julia M. Link[1,2], and Carsten Timm[1,2] — [1]Institute of Theoretical Physics, TU Dresden, 01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany

Noncentrosymmetric superconductors can support flat bands of zero-energy surface states in part of their surface Brillouin zone. This requires that they obey time-reversal symmetry and have a sufficiently strong triplet-to-singlet-pairing ratio to exhibit nodal lines in the bulk. These bands are protected by a winding number that relies on chiral symmetry, which is realized as the product of time-reversal and particle-hole symmetry. We reveal a way to stabilize a flat band in the entire surface Brillouin zone, while the bulk dispersion is fully gapped. The necessary ingredient is an additional spin-rotation symmetry that forces the direction of the spin-orbit-coupling vector not to depend on the momentum component normal to the surface. We define a winding number which leads to flat zero-energy surface bands. In addition, we consider how a weak breaking of the additional symmetry affects the surface band, employing first-order perturbation theory and a quasiclassical approximation.

TT 36.7 Wed 11:00 H 3005

Exceeding the Chandrasekhar-Clogston limit in flat-band superconductors: A multiband strong-coupling approach —

•Kristian Maeland and Asle Sudbø — Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

Hybrid systems of superconductors and magnets display promising applications in superconducting spintronics. This motivates a search for systems where superconductivity can survive larger in-plane critical magnetic fields than the conventional limit. The Chandrasekhar-Clogston (CC) limit applies to thin-film conventional superconductors with in-plane magnetic fields. For a magnetic field strength comparable to the superconducting gap, a spin-split normal state attains lower free energy than the superconducting state. A multiband superconductor with a flat band placed just below the Fermi surface has been shown to surpass the CC limit using weak-coupling theory. It is natural to anticipate corrections from strong-coupling theory in flat-band systems, owing to the large density of states of the flat bands. We derive Eliashberg equations and the free energy for a multiband superconductor in a magnetic field. First, we show that the CC limit can be exceeded by a small amount in one-band strong-coupling superconductors due to self-energy renormalization of the magnetic field. Next, we consider a two-band system with one flat band and find that the CC limit can be exceeded by a large amount also in strong-coupling theory, even when including hybridization between bands that intersect. [1] arXiv:2310.03082

15 min. break

TT 36.8 Wed 11:30 H 3005

Theory of superconductivity in thin films under an external electric field — •Alessio Zaccone[1] and Vladimir Fomin[2,3] — [1]University of Milan, Department of Physics, Milan, Italy — [2]Leibniz IFW Dresden, Germany — [3]Department of Theoretical Physics Moldova State University, Republic of Moldova

The supercurrent field effect is experimentally realized in various nanoscale devices, based on the superconductivity suppression by external electric fields being effective for confined systems. In spite of intense research, a microscopic theory and explanation of this effect is missing. Here, a microscopic theory of superconductivity in thin films is presented, which accounts for the effect of quantum confinement on the electronic density of states, on the Fermi energy, and on the topology of allowed states in momentum space. By further accounting for the interplay between quantum confinement, the external static electric field, the Thomas-Fermi screening in the electron-phonon matrix element, and the effect of confinement on the Coulomb repulsion parameter, the theory predicts the critical value of the external electric field as a function of the film thickness, above which superconductivity is suppressed. In particular, this critical value of the electric field is the lower the thinner the film, in agreement with recent experimental observations. Crucially, this effect is predicted by the theory when both Thomas-Fermi screening and the Coulomb pseudopotential are taken into account, along with the respective depencence on thin film thickness. This microscopic theory of the supercurrent field-effect opens up new possibilities for electric-field gated quantum materials.

TT 36.9 Wed 11:45 H 3005

Superconductivity due to fluctuating loop currents — Grgur Palle[1], •Risto Ojajärvi[1], Rafael M. Fernandez[2], and Jörg Schmalian[1,3] — [1]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA — [3]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Orbital magnetism and the loop currents (LC) that accompany it have been proposed to emerge in many systems, including cuprates, iridates, and kagome superconductors. In the case of cuprates, LCs have been put forward as the driving force behind the pseudogap, strange-metal behavior, and $d_{x^2-y^2}$-wave superconductivity. Here, we investigate whether fluctuating intra-unit-cell loop currents can cause unconventional superconductivity. For odd-parity LCs, we find that they are strongly repulsive in all pairing channels near the underlying quantum-critical point (QCP). For even-parity LCs, their fluctuations do give rise to unconventional pairing. However, this pairing is not amplified in the vicinity of the QCP, in sharp contrast to other known cases of pairing mediated by intra-unit-cell order parameters, such as spin-magnetic, nematic, or ferroelectric ones. Applying our formalism to the cuprates, we conclude that pairing mediated by fluctuating intra-unit-cell LCs is unlikely to yield $d_{x^2-y^2}$-wave superconductivity. We also show that loop currents, if relevant for the cuprates, must vary between unit cells and break translation symmetry.

TT 36.10 Wed 12:00 H 3005

Electronic theory for FFLO state in iron-based superconductors: role of spin-orbit coupling and pairing symmetry — •Luka Jibuti and Ilya Eremin — Rurh universität Bochum, Bochum, Germany

We develop an electronic theory of the existence and the mannerisms of the Fulde-Ferrel-Larkin-Ovchinnikov(FFLO) phase in the multiorbital iron-based superconductors. The starting point is the low energy Hamiltonian including realistic description of the spin-orbit coupling, correctly describing the Fermi surfaces of various types of iron-based superconductors. We first address the formation of FFLO state in the in-plane magnetic field in strongly hole- and electron-doped systems such as KFe2As2 and electron intercalated FeSe compounds, respectively. We also show that the formation of the FFLO state is unlikely for the s+- superconducting state in the situation when both electron and hole pockets are present at the Fermi level due to effect of the spin-orbit coupling.

TT 36.11 Wed 12:15 H 3005

Zero-field finite-momentum and field-induced superconductivity in altermagnets — •Debmalya Chakraborty and Annica M. Black-Schaffer — Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden

We explore the possibilities for spin-singlet superconductivity in newly discovered altermagnets. Investigating d-wave altermagnets, we show that finite-momentum superconductivity can easily emerge in altermagnets even though they have no net magnetization, when the superconducting order parameter also has d-wave symmetry with nodes coinciding with the altermagnet nodes. Additionally, we find a rich phase diagram when both altermagnetism and an external magnetic field are considered, including superconductivity appearing at high magnetic fields from a parent zero-field normal state.

TT 36.12 Wed 12:30 H 3005

Proximity-induced gapless superconductivity in two-dimensional Rashba semiconductor in magnetic field — •Serafim Babkin[1], Andrew Higginbotham[1,2], and Maksym Serbyn[1] — [1]Institute of Science and Technology Austria (ISTA), Am Campus 1, 3400 Klosterneuburg, Austria — [2]The James Franck Institute and Department of Physics, University of Chicago, Chicago, Illinois 60637, USA

Two-dimensional semiconductor-superconductor heterostructures form the foundation of numerous nanoscale physical systems. However, measuring the properties of such heterostructures, and characterizing the semiconductor in-situ is challenging. Motivated by experiments, we introduce a theoretical model describing a disordered semiconductor with strong spin-orbit coupling that is proximitized by a superconductor. Our model provides specific predictions for the density of states and superfluid density. Presence of disorder leads to the emergence of a gapless superconducting phase, that may be viewed as a manifestation of Bogoliubov Fermi surface. When applied to real experimental data, our model showcases excellent quantitative agreement, enabling the extraction of material parameters such as mean free path and mobility, and estimating g-tensor after taking into account the orbital contribution of magnetic field. Our model can be used to probe in-situ parameters of other superconductor-semiconductor heterostructures and can be further extended to give access to transport properties.

TT 36.13 Wed 12:45 H 3005

Singlet-Triplet Mixing, Topological Superconductivity and Topological Phase Transitions in the Triangular-Lattice Rashba Hubbard model — •Matthew Bunney[1,2], Jacob Beyer[1,2,3,4], Carsten Honerkamp[2,3], and Stephan Rachel[1] — [1]School of Physics, University of Melbourne, Parkville, VIC 3010, Australia — [2]Institute for Theoretical Solid State Physics, RWTH Aachen University, 52062 Aachen, Germany — [3]JARA Fundamentals of Future Information Technology, 52062 Aachen, Germany — [4]Institute for Theoretical Physics, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

The superconducting phase diagram of the triangular-lattice Rashba Hubbard model in the absence of spin-orbit coupling features at very low fillings triplet superconductivity but otherwise singlet d-wave superconductivity, ubiquitous on two-dimensional hexagonal lattices. In the presence of spin-orbit coupling, the mixing of singlet and triplet pairings can be analysed within truncated-unity functional renormalization group (TU-FRG). By combining group theoretical arguments with extensive TU-FRG simulations, we show that a phase with two-dimensional E_2 irrep prevails. However, by analysing the TU-FRG results further, we find that this phase splits into various topological superconducting phases, separated by topological phase boundaries. Our work positions TU-FRG as a method which can resolve structure within the otherwise uniform many-electron phases.