TT 50: Superconductivity: Theory II

Time: Wednesday 15:00–18:00 Location: H 3005

TT 50.1 Wed 15:00 H 3005

Floquet engineering Higgs dynamics in superconductors — •Tobias Kuhn[1], Björn Sothmann[2], and Jorge Cayao[3] — [1]Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Physics, University of Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany — [3]Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden

The order parameter Δ of periodically driven superconductors with frequency Ω shows spontaneous symmetry breaking analogue to Higgs mechanism [1]. The resulting Higgs mode can be resonantly excited in subgap regime at $\Omega = \Delta$ through non-linear coupling to light [2]. We develop a Floquet approach to study Higgs dynamics captured by anomalous Floquet Green's functions. This description exploits the drives periodicity to considerably reduce the complexity of the time-dependent problem [3]. Interestingly, the Floquet approach naturally offers a physical explanation for the renormalized steady state order parameter as a result of photon processes between Floquet subbands. As an example, we demonstrate Floquet engineering Higgs modes in time-periodic s-wave superconductors. Notably, the theory can easily be extended to spin-triplet superconductors and complex interactions as well.

[1] R. Shimano, N. Tsuji, Annu. Rev. Condens. Matter Phys. **11** (2020) 103
[2] N. Tsuji, H. Aoki, Phys. Rev. B **92** (2015) 064508
[3] J. Cayao, C. Triola, A. M. Black-Schaffer, Phys. Rev. B **103**, 104505 (2021).

TT 50.2 Wed 15:15 H 3005

Theory of Superconductors in non-equilibrium: response of the Higgs mode — •Sida Tian[1], Rafael Haenel[1,2], and Dirk Manske[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver V6T 1Z4, Canada

Collective modes in superconductors encode rich information about the superconducting state. Experimentally probing them requires THz lasers that push the system away from equilibrium. Here we present a response theory based on Keldysh formalism that allows one to capture the dynamics of a superconductor in the non-equilibrium regime. The method is based on a generalisation of the Kubo formula, and compute the response of a non-equilibrium state subject to a small external perturbation. Because of this, we can also isolate contributions from different channels to the electromagnetic response kernel. This theory allows one to capture phenomena in pump-probe experiment beyond Matsubara formalism, and gives insight into the dynamics of superconductors away from equilibrium.

TT 50.3 Wed 15:30 H 3005

Non-equilibrium THz response of time-reversal symmetry breaking superconductors — •Silvia Neri and Dirk Manske — Max Planck Institute for Solid State Research D-70569, Stuttgart, Germany

Time-reversal symmetry breaking (TRSB) superconductors are unconventional superconductors that show a rich collective mode spectra. These collective excitations in superconductors provide crucial information of the symmetry broken phase, in particular, serving as a fingerprint for determining the ground state gap symmetry. In this work we consider multiple TRSB superconductors characterized by an order parameter of the form $\Delta = \Delta_1 + i\Delta_2$. We provide a classification scheme of the collective excitations in the above systems as a function of the ratio between the components Δ_1/Δ_2. In order to excite the many modes in the systems we have adopted two different probes: a quench symmetry of the condensate and a finite momentum transfer induced by an external electric field. Both methods allow us to excite and identify the different modes in the spectra. Furthermore, we have numerically simulated the response resulting from an excitation scheme mimicking a pump-prob experimental scenario. We have calculated the transient optical response identifying and classifying the resulting spectra also in terms of the component ratio. Our classification could provide a way to distinguish between different order parameters symmetries of a TRSB superconducting condensate and estimate the magnitude of the different components constituting the sample.

TT 50.4 Wed 15:45 H 3005

Nonthermal superconductivity in photodoped multiorbital Hubbard systems — •Sujay Ray — University of Fribourg, 1700 Fribourg, Switzerland

Superconductivity in laser-excited correlated electron systems has attracted considerable interest due to reports of light-induced superconductinglike states. Here we explore the possibility of nonthermal superconducting order in strongly interacting multiorbital Hubbard systems, using nonequilibrium dynamical mean field theory. We find that a staggered η-type superconducting phase can be realized on a bipartite lattice in the high photodoping regime, if the effective temperature of the photocarriers is sufficiently low. The η superconducting state is stabilized by Hund coupling - a positive Hund coupling favors orbital-singlet spin-triplet η pairing, whereas a negative Hund coupling stabilizes spin-singlet orbital-triplet η pairing.

TT 50.5 Wed 16:00 H 3005

Nonequilibrium quasiparticle distribution in superconducting resonators: effect of pair-breaking photons — •Paul Benedikt Fischer[1,2] and Gianluigi Catelani[1,3] — [1]JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany — [3]Quantum Research Center, Technology Innovation Institute, Abu Dhabi 9639, UAE

In the superconducting state, the presence of the finite gap in the excitation spectrum implies that the number of excitations (quasiparticles) is exponentially small at temperatures well below the critical one. Nevertheless, experiments at low temperature usually find a finite, non-negligible density of quasiparticles whose origin has been attributed to various non-equilibrium phenomena. Here, we investigate the role of photons with energy exceeding the pair-breaking threshold 2Δ as a possible source for these quasiparticles in superconducting resonators. Modeling the interacting system of quasiparticles, phonons, sub-gap and pair-breaking photons using a kinetic equation approach, we find analytical expressions for the quasiparticles' density and their energy distribution. Applying our theory to measurements of quality factor as function of temperature and for various powers, we find they could be explained by assuming a small number of photons above the pair-breaking threshold.

TT 50.6 Wed 16:15 H 3005

High-T$_c$ phononic superconductivity at room pressure: Insights from ab initio simulations — •Antonio Sanna[1], Camilla Pellegrini[1], Miguel A. L. Marques[2], and Tiago Cerqueira[3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]CFisUC, Department of Physics, University of Coimbra, Portugal — [3]Ruhr University Bochum, Germany

The recent discovery of near room temperature conventional superconductivity at high pressure has triggered an intense search for new phonon-mediated superconductors, which is driven and led by modern computational techniques.

While room temperature and even hot-superconductivity appears to be likely possible under pressure, it is not yet clear if these extreme superconducting states can be achieved at room pressure.

We present the ab initio SCDFT and Eliashberg[1,2] characterization of several superconductors which have been predicted by means of an extensive high throughput scan involving over 200 000 stable or nealy-stable metallic compounds[3]. Although none of the predicted materials have critical temperatures above 100K, several are comparable or even superior to MgB_2. The analysis of these materials and the extensive high throughput data is used to estimate the likelihood of finding new technologically useful phononic superconductors via high-throughput search.

[1] Sanna et al., Phys. Rev. B 108 (2023) 064511
[2] Pellegrini et al., J. Phys. Mater. 5 (2022) 024007
[3] Cerqueira et al., adma.202307085 (2023)

15 min. break

TT 50.7 Wed 16:45 H 3005

Ab initio calculations of superconducting transition temperatures beyond GW-RPA — •Camilla Pellegrini[1], Carl

Kukkonen[2], and Antonio Sanna[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]33841 Mercator Isle, Dana Point, California 92629, USA

In ab initio calculations of superconducting properties, the Coulomb repulsion is accounted for at the GW level [1,2] and is usually computed in the random phase approximation (RPA), which neglects vertex corrections both at the polarizability level and in the self-energy. Although this approach is unjustified, the brute force inclusion of higher-order self-energy corrections is computationally prohibitive.

We propose a generalized GW self-energy, where vertex corrections are incorporated into W by employing the Kukkonen and Overhauser (KO) ansatz for the effective interaction between two electrons in the electron gas [3]. By computing the KO interaction in the adiabatic local density approximation, and using it in the Eliashberg equations, we find that vertex corrections lead to a systematic decrease of the critical temperature (T_c), ranging from a few percent in bulk lead to more than 40

[1] C. Pellegrini, R. Heid, A. Sanna, J. Phys. Mater. 5 (2022) 024007
[2] A. Sanna, C. Pellegrini, E.K.U. Gross, Phys. Rev. Lett. 125 (2020) 057001
[3] C. Pellegrini, C. Kukkonen, A. Sanna, Phys. Rev. B 108 (2023) 064511

TT 50.8 Wed 17:00 H 3005

Bypassing the BCS-to-BEC crossover in strongly correlated superconductors: resilient coherence from multiorbital physics — •Niklas Witt[1,2], Yusuke Nomura[3], Sergey Brener[1], Ryotaro Arita[4,5], Alexander I. Lichtenstein[1,2], and Tim Wehling[1,2] — [1]University of Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Germany — [3]Keio University, Japan — [4]University of Tokyo, Japan — [5]RIKEN CEMS, Japan

Superconductivity emerges from the spatial coherence of a macroscopic condensate of Cooper pairs. Increasingly strong binding and localization of electrons into these pairs compromises the condensate's phase stiffness, thereby limiting critical temperatures – a phenomenon commonly known as the BCS-to-BEC crossover. In this study [1], we report on the circumvention of the BCS-BEC crossover present in a multi-orbital model of alkali-doped fullerides (A_3C_{60}). Our findings reveal a localized superconducting regime characterized by a robustly short coherence length and a domeless rise in critical temperature with increasing pairing interaction. We identify strong correlations and multi-orbital effects as the underlying cause of this behavior. These insights are derived from the development of a theoretical framework to calculate the fundamental intrinsic length scales of superconductors, namely the coherence length (ξ_0) and the London penetration depth (λ_L). Importantly, our approach allows for the determination of these scales in microscopic theories and from first principles, even in the presence of strong electron correlations.

[1] N. Witt et al., arXiv:2310.09063 (2023)

TT 50.9 Wed 17:15 H 3005

Splitting of d-wave surface states: Edge ferromagnetism or spontaneous supercurrents? — •Kevin Marc Seja, Niclas Wall-Wennerdal, Tomas Löfwander, and Mikael Fogelström — MC2 - Microtechnology & Nanoscience, Chalmers University of Technology, Gothenburg, Sweden

At pair-breaking surfaces of a d-wave superconducting grain, Andreev bound states appear in the middle of the superconducting energy gap. The resulting large density of states at zero energy is energetically highly unfavorable. Experimentally, the associated tunneling-conductance peak was found to split spontaneously into two finite-energy peaks at low temperatures[1]. Two suggested mechanisms for this are either ferromagnetic interaction at the surfaces[2], or the establishment of phase gradients in the order parameter[3]. It is an open question which of the two cases minimizes the free energy at finite temperatures. Here we present a theoretical study of this problem using the quasiclassical theory of superconductivity. We include a magnetic Fermi liquid interaction, allow for a complex order parameter, and solve the underlying transport and self-energy equations selfconsistently in 2D by finite element method[4]. Depending on interaction strength and temperature, we find either a first-order transition to a purely magnetic or a second-order transition to a current-carrying state. We discuss key differences between the two phases.

[1] Covington et al., Phys. Rev. Lett. 79 (1997) 277
[2] Potter & Lee - Phys. Rev. Lett. 112 (2014) 117002
[3] Håkansson et al., Nat. Phys. 11 (2015) 755
[4] Seja & Löfwander - Phys. Rev. B 106 (2022) 144511

TT 50.10 Wed 17:30 H 3005

Shedding light on collective modes in 2D superconductors — •Benjamin Levitan[1,2], Erez Berg[1], Yuval Oreg[1], Mark Rudner[3], and Ivan Iorsh[1,4] — [1]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel — [2]Institute for Theoretical Physics, University of Köln, Köln, Germany — [3]Department of Physics, University of Washington, Seattle, WA, USA — [4]Department of Physics, Engineering Physics and Astronomy, Queen's University, Kingston, Ontario, Canada

The order parameter of a conventional single-band superconductor, being a complex number, lives in a two-dimensional configuration space. Accordingly, there are always at least two collective excitation modes associated with superconducting order: the condensate may fluctuate in amplitude or overall phase. In unconventional superconductors, finer order-parameter structure and/or subdominant pairing channels can provide additional directions in which fluctuations may occur, yielding a richer spectrum of collective modes.

I will discuss our theoretical study of the collective modes in two-dimensional unconventional superconductors, using rhombohedral trilayer graphene (RTG) as an illustrative case study. RTG hosts an annular Fermi sea prior to the onset of superconductivity; I will show how the two Fermi surface components can give rise to an in-gap Leggett mode in the superconducting state. I will then show how the linear absorption spectrum for AC out-of-plane displacement fields can yield insight into the superconducting gap structure, and even into the nature of the underlying microscopic interactions responsible for pairing.

TT 50.11 Wed 17:45 H 3005

Fractal superconductivity — •Robert Canyellas — Institute for Molecules and Materials, Radboud University, Heyendaalseweg 135, 6525AJ Nijmegen, The Netherlands

Fractal structures such as the Sierpinski gasket have been theoretically predicted to enhance the critical temperature of superconductivity, as compared with regular crystals, while maintaining the macroscopic phase coherence of the Cooper pairs. Before, the analysis has been performed for the s-wave attractive Hubbard model. In our work, we extend it to the different types of pairing symmetries, such as p and d-wave, for the extended attractive Hubbard model on the Sierpinski gasket and carpet geometries. We use the Bogoliubov-de Gennes mean field theory and the kernel polynomial method implementation to compute the spatial profile of the order parameter and the superfluid density, and derive the phase diagram of the system.