TT 63: Superconductivity: Theory

Time: Friday 9:30–13:15 Location: HSZ 103

TT 63.1 Fri 9:30 HSZ 103

Sharp Kohn-like phonon anomalies due to charge order can strongly enhance the superconducting T_c — •Alessio Zaccone — Department of Physics, University of Milan, 20133 Milano, Italy

Phonon softening is a ubiquitous phenomenon in condensed matter systems which is usually associated with charge density wave (CDW) instabilities and anharmonicity. The interplay between phonon softening, CDW and superconductivity is a topic of intense debate. In this work, the effects of anomalous soft phonon instabilities on superconductivity are studied based on a recently developed theoretical framework that accounts for phonon damping and softening within the Migdal-Eliashberg theory [1]. Model calculations [2] show that the phonon softening in the form of a dip in the phonon dispersion relation, either acoustic or optical (including the case of Kohn-type anomalies typically associated with CDW), can cause a manifold increase of the electron-phonon coupling constant λ. This, under certain conditions, which are consistent with the concept of optimal frequency introduced by Bergmann and Rainer, can produce a large increase of the superconducting transition temperature T_c. These results suggest the possibility of reaching high-temperature superconductivity by exploiting soft phonon anomalies restricted in momentum space.
[1] M. Baggioli, C. Setty, A. Zaccone, Phys. Rev. B 101, 214502 (2020)
[2] arXiv:2211.12015v2

TT 63.2 Fri 9:45 HSZ 103

Universal suppression of superfluid weight by non-magnetic disorder in s -wave superconductors independent of quantum geometry and band dispersion — •Alexander Lau[1], Sebastiano Peotta[2], Dmitry I. Pikulin[3], Enrico Rossi[4], and Timo Hyart[1,2] — [1]MagTop, IF PAN, Warsaw, Poland — [2]Aalto University, Finland — [3]Microsoft Quantum, Redmond, USA — [4]William & Mary, Williamsburg, USA

Motivated by the experimental progress in controlling the properties of the energy bands in superconductors, significant theoretical efforts have been devoted to study the effect of the quantum geometry and the flatness of the dispersion on the superfluid weight. In conventional superconductors, where the energy bands are wide and the Fermi energy is large, the contribution due to the quantum geometry is negligible, but in the opposite limit of flat-band superconductors the superfluid weight originates purely from the quan- tum geometry of Bloch wave functions. Here, we study how the energy band dispersion and the quantum geometry affect the disorder-induced suppression of the superfluid weight [1]. In particular, we consider non-magnetic disorder and s -wave superconductivity. Surprisingly, we find that the disorder-dependence of the superfluid weight is universal across a variety of models, and independent of the quantum geometry and the flatness of the dispersion. Our results suggest that a flat-band superconductor is as resilient to disorder as a conventional superconductor.
[1] SciPost Phys. 13, 086 (2022)

TT 63.3 Fri 10:00 HSZ 103

Correction to Morel-Anderson-Tolmachev pseudopotential from nonlocal Coulomb interaction in 2D superconductors — •Manuel Simonato, Malte Rösner, and Mikhail I. Katsnelson — Radboud University, Nijmegen, NL

The repulsive Coulomb interaction between electrons is detrimental to conventional superconductivity. The widely accepted model to account for this is to describe this repulsion with a purely local interaction of strength μ_C. Morel, Anderson, and Tolmachev then showed that the superconducting quantities are effectively described by a renormalized parameter μ_C^*, as a direct consequence of the energy scale separation between phonons and electrons. In 2D the screening properties are less efficient and modeling the Coulomb repulsion with a strictly local interaction can result in inaccurate description. We therefore study how superconducting properties are affected by nonlocal Coulomb repulsions. We find that the superconducting state can still be accurately described when a revised Coulomb pseudopotential $\tilde{\mu}_C^*$ is used. We show that the revised parameter, which accounts for nonlocal interactions, is always larger that the convetional μ_C^*. The non-local Coulomb interaction thus suppresses superconductivity and the critical temperature even further. Analyzing the Bethe-Salpeter equation describing the screening of Coulomb interaction in 2D, we obtain an analytical expression for $\tilde{\mu}_C^*$, and show that the structure of the nonlocal Coulomb interaction weakens the screening effects from high-energy pair fluctuations and therefore yields larger values of the pseudopotential.

TT 63.4 Fri 10:15 HSZ 103

Coherence and pairing fluctuations in strongly correlated superconductors — •Niklas Witt[1,2], Sergey Brener[1], Yusuke Nomura[3], Ryotaro Arita[4,5], Alexander 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

The fundamental properties of superfluids and superconductors are determined by the spatial coherence of the macroscopic condensate. Central to this characterization is the knowledge of the coherence length ξ, as it specifies the relevant length scales for fluctuations pertinent to, e.g., the formation of vortex latices or magneto-thermal transport. While the description of ξ is well established in weak-coupling BCS theory and Eliashberg-theory, it is a generally unknown quantity in strongly correlated superconductors, where spatiotemporal fluctuations influence the critical temperature [1] and might underlie light-induced enhancement of superconductivity [2].

In this work, we establish a link to directly calculate the coherence length for superconductors with strong electron correlations from microscopic theories and first principles. We illustrate with the example of Alkali-doped fullerides (A_3C_{60}) how proximity of superconducting and Mott-localized states impact superconducting coherence, pairing fluctuations, and critical temperature. Our analysis shows Eliashberg-type behavior of strongly correlated superconductors.
[1] Emery & Kivelson, Nature **374** (1995)
[2] Fausti et al., Science **331** (2011)
Mitrano et al., Nature **530** (2016)

TT 63.5 Fri 10:30 HSZ 103

Superconductivity from repulsive interactions due to strong-coupling to a Mott-insulating layer — •Clara S. Weber[1,2], Dante M. Kennes[1], and Martin Claassen[2] — [1]RWTH Aachen, Aachen, Germany — [2]University of Pennsylvania, Philadelphia, USA

While superconductors in their conventional form are established by effective attractive interactions, mechanisms for emergent electronic pairing from strong repulsive electron-electron interactions remain under considerable debate. Here, we establish a strong-coupling mechanism that realizes intertwined superconductivity and magnetic order in a Kondo-like bilayer system with purely repulsive interactions, composed of a two-dimensional Mott insulator with strong Hubbard interactions coupled to a layer of weakly-interacting itinerant electrons. Remarkably, this model allows for a rigorous strong-coupling analysis, where we find that itinerant electrons in the nearly-metallic layer are subject to an effective attractive electron-electron interaction as a function of magnetic ordering in the Mott-insulating layer. We carefully study this behavior numerically using large scale DMRG calculations and find that the superconducting behavior persists in a wide parameter range beyond the strong-coupling regime. Additionally, we classify the rich magnetic phase diagram and find a 2-site antiferromagnetic and a 4-site antiferromagnetic phase, along with a phase separation regime. Finally, we discuss possible applications and realizations of the proposed mechanism.

TT 63.6 Fri 10:45 HSZ 103

Simulating superconducting properties of overdoped cuprates: The role of inhomogeneity — Mainak Pal[2], •Andreas Kreisel[1], William A. Atkinson[3], and Peter J. Hirschfeld[2] — [1]Niels Bohr Institute, University of Copenhagen, Denmark — [2]Department of Physics, University of Florida, USA — [3]Department of Physics and Astronomy, Trent University, Canada

Theoretical studies of disordered d-wave superconductors have focused, with a few exceptions, on optimally doped models with strong scatterers. Addressing recent controversies about the nature of the overdoped cuprates, however, requires studies of the weaker scattering associated with dopant atoms. Here we study simple models of such systems in the self-consistent Bogoliubov-de Gennes (BdG) framework, and compare to disorder-averaged results using the self-consistent-T-matrix-approximation (SCTMA). Despite surprisingly linear in energy

behavior of the low-energy density of states even for quite disordered systems, the superfluid density in such cases retains a quadratic low-temperature variation of the penetration depth, unlike other BdG results reported recently. We trace the discrepancy to smaller effective system size employed in that work. Overall, the SCTMA performs remarkably well, with the exception of highly disordered systems with strongly suppressed superfluid density. We explore this interesting region where gap inhomogeneity dominates measured superconducting properties, and compare with overdoped cuprates.

[1] M. Pal, A. Kreisel, W.A. Atkinson, P.J. Hirschfeld arXiv:2211.13338 (2022)

TT 63.7 Fri 11:00 HSZ 103

Finite energy Cooper pairing in multiband superconductors — •Masoud Bahari[1], Song-Bo Zhang[2], Chang-An Li[1], Sang-Jun Choi[1], Carsten Timm[3], and Björn Trauzettel[1] — [1]University of Würzburg, Würzburg, Germany — [2]University of Zürich, Zürich, Switzerland — [3]Technische Universität Dresden, Dresden, Germany

Extensive efforts have been carried out to understand the superconducting pairing symmetry since the birth of Bardeen-Cooper-Schrieffer theory. In weakly interacting systems, the essential ingredient is a weak effective electron-electron interaction at the Fermi energy resulting in particular bulk properties including superconducting gaps possibly with nodes.

We demonstrate and discuss the bulk and surface spectral properties of a novel pairing mechanism that occurs at finite excitation energies in multiband superconductors. In the bulk, it is manifested by the appearance of superconducting coherence peaks in the density of states at finite energies. Interestingly, on the surface, we predict the emergence of a pair of helical topological Dirac surface cones when the finite energy pairing is odd-parity.

Finally, we propose aluminum in proximity with (111) surface of gold to realize the bulk properties of finite energy pairing. We discuss the pairing symmetry of the system by employing the density-functional theory, and an analytical model based on the Bogoliubov-de Gennes formalism. The signature of such a pairing gives important information about the correct pairing symmetry of a superconductor.

15 min. break

TT 63.8 Fri 11:30 HSZ 103

Fragmented Cooper pair condensation in striped superconductors — •Alexander Wietek — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, Dresden 01187, Germany

Condensation of bosons in Bose-Einstein condensates or Cooper pairs in superconductors refers to a macroscopic occupation of a few single- or two-particle states. A condensate is called *fragmented* if not a single, but multiple states are macroscopically occupied. While fragmentation is known to occur in particular Bose-Einstein condensates, we propose that fragmentation naturally takes place in striped superconductors. To this end, we investigate the nature of the superconducting ground state realized in the two-dimensional t*t**J model. In the presence of charge density modulations, the condensate is shown to be fragmented and composed of partial condensates located on the stripes. The fragments of the condensates hybridize to form an extended macroscopic wave function across the system. The results are obtained from evaluating the singlet-pairing two-particle density matrix of the ground state on finite cylinders computed via the density matrix renormalization group method. Our results shed light on the intricate relation between stripe order and superconductivity in systems of strongly correlated electrons.

TT 63.9 Fri 11:45 HSZ 103

Superconductivity on the honeycomb lattice: A truncated unity perspective — •Matthew Bunney[1,2], Jacob Beyer[1,2], Carsten Honerkamp[2], and Stephan Rachel[1] — [1]School of Physics, University of Melbourne, Melbourne, Australia — [2]Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany

The honeycomb lattice provides one of the simplest scenarios with sublattice degrees of freedom. For Cooper pairing of electrons on this lattice, this opens extensive and intricate opportunities of interplay between the momentum space wavefunction, the electron spins and the orbital (sublattice) dependencies. Recent advances and improvements in truncated unity versions of the functional renormalization group allows us to fully capture these phenomena. We thus revisit the honeycomb Hubbard model and its electron pairing and density wave instabilities. A particular emphasis is placed on the formation of sublattice singlets and the resulting exotic pairing states.

TT 63.10 Fri 12:00 HSZ 103

A low-dimensional ML Surrogate Model for Critical Temperature Prediction of Superconductors — •Angel Diaz Carral[1], Martin Roitegui Alonso[1], and Maria Fyta[2] — [1]Institute for Computational Physics, Universität Stuttgart, Allmandring 3, 70569, Stuttgart, Germany — [2]Computational Biotechnology, RWTH-Aachen University, Worringerweg 3, 52074, Aachen, Germany

A general theory of superconductivity has been the focus of research over the last decades. Machine learning (ML) approaches based on chemical and structural features have been developed in order to predict both the critical temperature (Tc) and potential novel superconducting structures. Nevertheless, the applied ML models lack interpretability; either the feature matrix is reduced via SVD/PCA transformations or augmented with statistical feature generation. Here, we introduce a ML model based only on electronic descriptors derived from the composition formula and the individual elements. We reach a very high accuracy (R2 over 91%) using a considerably reduced descriptor dimensionality, while retaining the physical meaning of the feature space. Our active learning model is efficiently tested in predicting critical temperatures and links to the discovery of new superconducting structures.

TT 63.11 Fri 12:15 HSZ 103

Ab initio study of magnetic doping in an Ising superconductor — •Mohammad Hemmati[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]University of Würzburg, Germany

The transition-metal dichalcogenide $NbSe_2$ is a layered superconducting material that exhibits unconventional Ising superconductivity that is particularly robust to certain directions of external magnetic fields [1]. We combined the Bogoliubov-de-Gennes formalism in the Korringa-Kohn-Rostoker Green function method with the Coherent Potential Approximation [2,3], to study superconducting $NbSe_2$ in the presence of dilute concentrations of magnetic transition-metal impurities. The ab initio results show a suppression of superconductivity at higher magnetic impurity concentration, which is in agreement with the Abrikosov-Gorkov theory.

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[1] K. S. Novoselov *et al.*, Science **353**, aac9439 (2016)
[2] https://jukkr.fz-juelich.de
[3] P. Rüßmann and S. Blügel, PRB **105**, 125143 (2022)

TT 63.12 Fri 12:30 HSZ 103

Chiral surface superconductivity in half-Heusler semimetals — •Tilman Schwemmer[1], Domenico Di Sante[2,3], Jörg Schmalian[4], and Ronny Thomale[1] — [1]Institute for Theoretical Physics, University of Wuerzburg, D-97074 Wuerzburg, Germany — [2]Department of Physics and Astronomy, University of Bologna, 40127 Bologna, Italy — [3]CCQ, Flatiron Institute, New York, NY 10010, USA — [4]Institute for Theory of Condensed Matter and Institute for Quantum Materials and Technologies, KIT, Karlsruhe 76131, Germany

We propose the metallic and weakly dispersive surface states of half-Heusler semimetals as a possible domain for the onset of unconventional surface superconductivity ahead of the bulk transition. Using density functional theory (DFT) calculations and the random phase approximation (RPA), we analyse the surface band structure of LuPtBi and its propensity towards Cooper pair formation induced by screened electron-electron interactions in the presence of strong spin-orbit coupling. Over a wide range of model parameters we find a chiral superconducting condensate featuring Majorana edge modes to be favoured energetically, while low-dimensional order parameter fluctuations trigger time-reversal symmetry breaking preceding the superconducting transition.

TT 63.13 Fri 12:45 HSZ 103

Transport in superconducting heterostructures: Quasiclassical theory and finite element method — •Kevin Marc Seja

and Tomas Löfwander — Department of Microtechnology and Nanoscience - MC2, Chalmers University of Technology, Gothenburg, Sweden

We present results on steady-state transport in mesoscopic conventional and unconventional superconductors coupled to either normal-metal or superconducting reservoirs. Our self-consistent simulations are using nonequilibrium quasiclassical theory in the Eilenberger formulation which allows different order parameter symmetries at arbitrary mean free path. Previously we investigated the thermoelectric effect[1] and spectral rearrangements due to a voltage bias[2] in d-wave superconductors. These studies on nonequilibrium effects assumed translational invariance normal to the transport direction.

This talk will address the question of how to go beyond such quasi one-dimensional models and study superconducting hybrid structures in realistic device geometries. To this end we present a finite element method[3] for the self-consistent solution of the underlying quasiclassical transport equations in dimensions larger than one, and give examples of its application.

[1] Seja & Löfwander, Phys. Rev. B 105, 104506 (2022)
[2] Seja & Löfwander, J. Phys.: Condens. Matter 34, 425301 (2022)
[3] Seja & Löfwander, Phys. Rev. B. 106, 144511 (2022)

TT 63.14 Fri 13:00 HSZ 103

Nonlinear response of diffusive superconductors to ac electromagnetic Fields — •Pascal Derendorf, Anatoly Volkov, and Ilya Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany

Using the generalized Usadel equation, we theoretically study the nonlinear response of a diffusive BCS superconductor to the action of electromagnetic fields. The response is found in the second order of the perturbation in the amplitude of the field E for the superconducting order parameter Δ and in the third order for the current j. We represent the matrix Keldysh function $\hat{g}^K$ as the sum of a regular function $\hat{g}^{reg}$ and an anomalous function $\hat{g}^{an}$. On the basis of this approach, general formulas for deviations of the retarded (advanced) Green's functions, as well as the Keldysh function for an arbitrary number of harmonics of the incident field are explicitly obtained. The frequency and temperature dependencies of zero harmonic $\delta\Delta_0$ (Eliashberg effect) and the second harmonic $\delta\Delta_{2\Omega}$ under action of a monochromatic irradiation are analyzed. We also study the third harmonic $j_{3\Omega}$ and the possibility of parametric amplification of a signal with a frequency Ω_x in the presence of a pumping with a frequency Ω which excites the Higgs (amplitude) mode.