TT 34: Superconductivity: Theory

Time: Wednesday 15:00–18:30 Location: H36

TT 34.1 Wed 15:00 H36

Eliashberg theory and band-off-diagonal superconductivity — •Bernhard Putzer[1,2] and Mathias S. Scheurer[1] — [1]Institute for Theoretical Physics III, University of Stuttgart, 70550 Stuttgart, Germany — [2]Institute for Theoretical Physics, University of Innsbruck, Innsbruck A-6020, Austria

In contrast to the mean field approximation of BCS theory, the Migdal-Eliashberg approach is a more sophisticated framework to describe phonon-mediated superconductivity. Allowing strong coupling between electronic and bosonic fields opens the door to investigate the effects of inter-band processes on the superconducting state in a controllable setting. We derive and solve the Eliashberg equations for a two-band model, inspired by twisted graphene systems, finding an entirely band-off-diagonal superconducting order parameter. By including full momentum and Matsubara fre- quency dependence, we uncover a mixing of even- and odd-frequency states induced by the band splitting. As a result, the superconductor exhibits very unconventional spectral properties for electron-phonon pairing; this includes a region with a nodal spectrum and a region with finite gap, which is, however, much smaller than the order parameter magnitude. Our findings have consequences for recent experiments on the superconducting state in twisted bilayer and trilayer graphene.

TT 34.2 Wed 15:15 H36

From charge fluctuations to pairing instabilities: Nonperturbative enhancement of the electron-phonon coupling driven by electronic correlations — •Emin Moghadas[1], Matthias Reitner[1], Alexander Kowalski[2], Giorgio Sangiovanni[2], Sergio Ciuchi[3,4], and Alessandro Toschi[1] — [1]Institute of Solid State Physics, TU Wien, Vienna, Austria — [2]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [3]Dipartimento di Scienze Fisiche e Chimiche, Università dell'Aquila, Coppito-L'Aquila, Italy — [4]Istituto dei Sistemi Complessi, CNR, Roma, Italy

We present a thorough investigation of the nonperturbative electronic mechanisms, which could lead to significant enhancements of the electron-phonon coupling in strongly correlated electron systems. Using dynamical mean-field theory (DMFT) for the single band Hubbard model on the square lattice, we analyze corrections to second-order electron-phonon processes arising from electronic fluctuations near the Mott metal-to-insulator transition (MIT). In this regime, the isothermal charge response becomes particularly large at small momenta, indicating tendencies towards phase-separation instabilities and enabling a substantial enhancement of the effective electron-phonon coupling. Eventually, we critically discuss the impact of our findings on observable spectral quantities as well as possible implications for the emergence of pairing instabilities.

TT 34.3 Wed 15:30 H36

Detailed analysis of the superconducting gap with Dynes pair-breaking scattering — •Anastasiya Lebedeva and František Herman — Comenius University in Bratislava

In our work, we study the energy gap behavior within the Dynes superconductor theory. This model generalizes the Bardeen-Cooper-Schrieffer (BCS) approach by including the pair-breaking disorder, introducing the tunneling in-gap states up to a Fermi level. Elaborating on the self-consistent gap equation, we obtain useful results which are also interesting from the experimental point of view. For example, the derived relations may serve to estimate the pair-breaking impurities concentration in the superconductor i.a. using only the energy gap and the critical temperature values of the material. Moreover, we offer the heuristic gap-to-temperature dependence providing up to 5%-precision in the whole temperature range. It is a more convenient tool compared to the cumbersome numerics used by now.

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TT 34.4 Wed 15:45 H36

Superconducting modes in the presence of Coulomb repulsion — •Joshua Althüser and Götz Uhrig — TU Dortmund, Otto-Hahn-Str. 4, 44227 Dortmund, Deutschland

We numerically study the collective excitations present in BCS-superconductors including screened Coulomb interactions. By varying the screening strength, we analyze its impact on the system. We use a formulation of the effective phonon-mediated interaction between electrons that depends on the energy transfer between particles, rather than being a constant in a small energy shell around the Fermi edge. We compute the system's Green's functions using the iterated equations of motion (iEoM) approach, which ultimately enables a comprehensive analysis of collective excitations. For weak couplings, we identify the well-known amplitude (Higgs) mode at the quasiparticle continuum's lower edge and the phase (Anderson-Bogoliubov) mode at zero energy for a neutral system, which shifts to higher energies as the Coulomb interactions are switched on. As the phononic coupling is increased, the Higgs mode emerges from the continuum, and additional phase and amplitude modes appear, persisting even with active Coulomb interactions.

TT 34.5 Wed 16:00 H36

Obstructed pairs with zero superfluid stiffness — •Tamaghna Hazra and Jörg Schmalian — Karslruhe Institute of Technology

We present a microscopic pairing mechanism in which the kinetic energy of pairs is much lower than the kinetic energy of electrons. This results in interaction-driven localization of charge without extrinsic disorder and is characterized by a vanishing superfluid stiffness. Localized pairs gain more kinetic energy from resonating between sublattices in a bosonic compact localized state, than from delocalizing throughout the material. This is grounded in a microscopic model building on a structural motif shared by many oxide superconductors - strongly interacting localized electrons realize spin degrees of freedom on the vertices and doped charge lives on the edges of the Bravais lattice. In the strong-coupling limit, local unconventional pairs realize the bosonic analogue of flat bands supported on line graphs. We discuss the experimental implications of this pairing mechanism, with concrete falsifiability criteria, and emphasize the broad scope of this recipe in connection to diverse families of strongly correlated materials which share the key ingredients that go into it.

TT 34.6 Wed 16:15 H36

Electronic structure and superconductivity in nickelates and cuprates: Insights from DMFT and DΓA — •Eric Jacob[1], Mario Malcolms de Oliveira[2], Thomas Schäfer[2], Paul Worm[1], Liang Si[3,1], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [3]School of Physics, Northwest University, Xi'an 710127, China

The infinite-layer nickelates and cuprates represent two compelling families of materials for exploring unconventional superconductivity and correlated electronic phenomena. I will discuss recent advances in understanding the electronic structure of infinite-layer nickelates, focusing on insights from dynamical mean-field theory (DMFT) and their comparison with experimental findings ([1]) from angle-resolved photoemission spectroscopy (ARPES). This helps [2] constrain possible scenarios for their electronic states. In particular, there is only one Ni orbital crossing the Fermi surface. Additionally, I will present ongoing investigations into superconductivity in both nickelates and cuprates, based on the dynamical vertex approximation ($D\Gamma A$ [3], [4]).

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[1] W. Sun et al., arXiv:2403.07344 (2024).
[2] L. Si et al., Phys. Rev. Res. 6, 043104 (2024).
[3] G. Rohringer et al., Rev. Mod. Phys. 90, 025003 (2018).
[4] M. Kitatani et al., J. Phys. Mater. 5, 034005 (2022).

TT 34.7 Wed 16:30 H36

Towards an *ab initio* theory of high-temperature superconductors: a study of multilayer cuprates. — •Benjamin Bacq-Labreuil[1,2], Benjamin Lacasse[1], André-Marie Tremblay[1], David Sénéchal[1], and Kristjan Haule[3] — [1]Institut quantique, Université de Sherbrooke, Canada — [2]IPCMS, Université de Strasbourg, France — [3]Center for Materials Theory, Rutgers University, USA

Significant progress towards a theory of high-temperature superconductivity in cuprates has been achieved via the study of effective models. Yet, material-specific predictions for high-temperature superconductors, while essential for constructing a comprehensive theory, remain out of reach. By combining cluster dynamical mean-field theory and density functional theory in a charge-self-consistent manner, here we show that the goal of material-specific predictions for high-temperature superconductors from first principles is within reach. We demonstrate the capabilities of our approach by performing an in-depth study of two representatives ($Ca_{(1+n)}Cu_nO_{2n}Cl_2$ and $HgBa_2Ca_{(n-1)}Cu_nO_{(2n+2)}$) of the still mysterious multilayer cuprates. We shed light on the microscopic origin of many salient features of multilayer cuprates, in particular the n-dependence of their superconducting properties. Our work establishes a framework for comprehensive studies of high-temperature superconducting cuprates, enables detailed comparisons with experiment, and, through its *ab initio* settings, unlocks opportunities for theoretical material design of high-temperature superconductors.

15 min. break

TT 34.8 Wed 17:00 H36

Enhanced entanglement in the pseudogap — •Frederic Bippus[1], Juraj Krsnik[1], Motoharu Kitatani[2,3], Anna Kauch[1], Gergö Roosz[4], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, Vienna, Austria — [2]Department of Material Science, University of Hyogo, Ako, Hyogo, Japan — [3]RIKEN Center for Emergent Matter Sciences (CEMS), Wako, Japan — [4]HUN-REN Wigner Research Centre for Physics, Budapest, Hungary

We show significantly enhanced entanglement in the pseudogap regime of the Hubbard model using the dynamical vertex approximation (DGA) [1], a non-local extension to the dynamical mean-field theory. The pseudogap, a partially gapped electronic state, is observed near the superconducting transition in cuprates and nickelates. Leveraging DGA, we compute the quantum variance-a lower bound to the quantum Fisher information [2] from the spin susceptibility directly on the imaginary Matsubara axis. By circumventing the need for ill-controlled analytical continuation, our approach provides a robust framework for probing entanglement depth. The results show good agreement with experimental data [3]. Additionally, Ornstein-Zernike fits provide analytical insights.

This work is supported by the SFB Q-M&S (FWF project ID F86).

[1] Rohringer et al., Rev. Mod. Phys., 90, 025003 (2018);
[2] Frérot et al., Phys. Rev. B, 94, 075121 (2016);
[3] Chan et al., Nat. Commun., 7, 10819 (2016).

TT 34.9 Wed 17:15 H36

Time evolution of surface state wave packets in nodal noncentrosymmetric superconductors — •Clara Johanna Lapp[1,2], Julia 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

Nodal noncentrosymmetric superconductors can host zero-energy flat bands of Majorana surface states within the projection of the nodal lines onto the surface Brillouin zone. Thus, these systems can have stationary, localized Majorana wave packets on certain surfaces, which may be a promising platfrom for quantum computation. However, for such applications it is important to find ways to manipulate the wave packets in order to move them without destroying their localization or coherence. As the surface states have a nontrivial spin polarization, applying an exchange field, e.g., by introducing a magnetic insulator at the surface, makes the previously flat band slightly dispersive. We aim to use an adiabatic change of the exchange field to move wave packets on the surface. We therefore investigate the time evolution of a maximally localized wave packet under the influence of such an exchange field employing exact diagonalization as well as quasiclassical approximations.

TT 34.10 Wed 17:30 H36

Interplay of superconductivity and altermagnetism: A symmetry perspective — •Kirill Parshukov[1], Niclas Heinsdorf[1,2], Benjamin T. Zhou[2], Marcel Franz[2], and Andreas P. Schnyder[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]The University of British Columbia, Vancouver BC, Canada

The interplay between altermagnetism and superconductivity gives rise to several interesting phenomena, including unconventional Josephson effects, diode effects, Cooper pair splitting, and topological superconductivity. In this talk, I investigate how altermagnetic symmetries can lead to new superconducting states with interesting topological properties. Since the superconducting gap functions must transform as irreducible co-representations of the spin-point groups, I first construct all possible superconducting basis functions. Importantly, because the spin-point group symmetries act simultaneously on the spin and the lattice, the spin and spatial parts of the basis functions are coupled in an intricate manner. I illustrate this by considering several examples in two dimensions, including the superconducting states of an altermagnet with four Dirac points [1].

[1] K. Parshukov, R. Wiedmann, A. P. Schnyder, arXiv:2403.09520.

TT 34.11 Wed 17:45 H36

Emergence of a condensate with finite-energy Cooper pairing in hybrid exciton/superconductor systems — •Viktoriia Kornich — University of Würzburg, Würzburg, Germany

I will consider a setup consisting of excitons formed in two valleys, with proximity-induced Cooper pairing, different in the conduction and valence bands. Due to the combination of a Coulomb interaction within excitons and superconducting proximity effects, Cooper pairing between electrons from valence and conduction bands from different valleys is formed. Thus, the gap between these electrons can be much larger than the usual superconducting pairing energies. This Cooper pairing has both even- and odd-frequency contributions. I will show that there is a phase transition into the formation of a robust macroscopic condensate of such Cooper pairs and then will suggest a detection scheme of it via Higgs modes.

TT 34.12 Wed 18:00 H36

Third-harmonic generation currents in pair-density wave superconductor — •Pascal Derendorf[1], Peayush Choubey[2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany — [2]Indian Institute of Technology-Roorkee, Roorkee, India

We investigate the signatures of a unidirectional pair-density wave (PDW) state in the third harmonic generation (THG) using an effective microscopic model, developed previously in Refs. [1,2]. The system possesses a unidirectional PDW state with d-wave symmetry in thermodynamic equilibrium ground state without extra need for an additional perturbation such as external Zeeman field or leading charge density wave order. We extend this model under the non-equilibrium by including a periodic driving in the form of external ac-field. The signatures of the emerging massive modes on the THG are derived via a gauge-invariant effective action approach. We discuss the emerging signatures in the third harmonic generation and their origin.

[1] F. Loder et al., Phys. Rev. B 81 (2010).
[2] J. Wårdh and M. Granath., Phys. Rev. B 96 (2017).

TT 34.13 Wed 18:15 H36

Describing superconductivity through interpretable artificial intelligence — •Herzain I. Rivera-Arrieta, Lucas Foppa, and Matthias Scheffler — The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Superconductivity is governed by an intricate interplay among electronic structure, lattice vibrations, and pressure effects, among many other phenomena [1]. Thus, a (single) physical model might not be enough to describe superconductivity. Interpretable artificial intelligence (AI) can provide valuable insights into the underlying mechanisms driving superconductivity, e.g., in conventional superconductors. Herein, we compile a dataset containing approximately 1,000 materials [2] and a diverse range of compositional, structural, electronic, and phonon-related properties. Then, we employ the symbolic-regression SISSO and subgroup discovery AI approaches [3, 4], to identify the few, key physicochemical parameters correlated with a superconductor's critical temperature. This approach is a step towards identifying the "materials genes" [5] of superconductivity.

[1] X. Gui, B. Lv, and W. Xie, *Chem. Rev.*, **121**, 2966 (2021).
[2] K. Choudhary, and K. Garrity, *Npj. Comut. Mater.*, **8**, 244 (2022).
[3] R. Ouyang, *et al.*, *Phys. Rev. Mat.*, **2**, 083802 (2018).
[4] S. Wrobel, *1st Europ. Symp. on Princ. of Data Min. and Knowl. Discov.*, **19**, 78 (1997).
[5] L. Foppa, *et al.*, *MRS bulletin*, **46**, 1016 (2021).