TT 99: Superconductivity: (General) Theory 2

Time: Thursday 15:00–18:00 Location: H 2053

TT 99.1 Thu 15:00 H 2053

Functional Development in Density Functional Theory for Superconductors — •Antonio Sanna, E.K.U. Gross, and Frank Essenberger — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

Density functional theory for superconductors (SCDFT) is a fully parameter-free approach to superconductivity that allows for accurate predictions of critical temperature and properties of superconductors. We report on the most recent extensions of the method, in particular the development of new functionals to:

1) incorporate in a correct fashion Migdal's theorem;
2) compute the excitation spectrum;
3) include spin-fluctuation mediated pairing

Applications and predictions are shown for a set of materials, including conventional and unconventional superconductors.

TT 99.2 Thu 15:15 H 2053

Coulomb interaction in Eliashberg theory of Superconductivity — •Arkadiy Davydov, Antonio Sanna, Sangeeta Sharma, John Kay Dewhurst, and Eberhard Gross — Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany

The Eliashberg theory [1] of superconductivity allows to describe materials with strong pairing interaction. In the non magnetic case it leads to a system of coupled integral multidimensional equations. Computational costs are usually reduced by an isotropic limit [2], and by restricting the Coulomb interaction to the use of one single parameter, μ^*, often chosen to give the experimental Tc. In this work we present the parameter-free approach in which the screened Coulomb interaction fully accounted within the Random Phase Approximation, entering the Eliashberg's equations on the same footing as the phononic interaction. We will compare this approach with Density Functional Theory for Superconductors [3, 4] where the corresponding approximation leads to a good agreement with experiments.

[1] G.M. Eliashberg, Sov. Phys. JETP 11, 696 (1960).
[2] D.J. Scalapino, Phys. Rev. 148, 263 (1966).
[3] L.N. Oliveira, E.K.U. Gross, Phys. Rev. Lett. 60, 2430 (1988).
[4] M. Lüders, PRB 72, 024545 (2005).

TT 99.3 Thu 15:30 H 2053

Superconductivity in intercalated group-IV honeycomb structures — •Jose A. Flores Livas and Antonio Sanna — Max-Planck-Institut für Mikrostrukturphysik. Weinberg 2, 06120. Halle (Saale) Germany.

We present in this talk a theoretical investigation on electron-phonon superconductivity of honeycomb MX_2 layered structures. Where X is one element of the group-IV (C, Si or Ge) and M an alkali or an alkaline-earth metal. Among the studied compositions we predict a T_c of 7 K in $RbGe_2$, 9 K in $RbSi_2$ and 11 K in SrC_2. Our SCDFT calculations evidence a strongly anisotropic superconducting gap, and the results show that despite the different doping and structural properties, the three families of materials fall into a similar description of its superconducting behavior. This allows us to estimate an upper critical temperature of about 20 K for the class of intercalated group-IV structures, including intercalated graphite and doped graphene.

TT 99.4 Thu 15:45 H 2053

Tuning non-equilibrium superconductors with lasers — •Michael A. Sentef[1], Alexander F. Kemper[2], Antoine Georges[3], and Corinna Kollath[1] — [1]HISKP, University of Bonn, Nussallee 14-16, D-53115 Bonn, Germany — [2]LBL Berkeley, USA — [3]Ecole Polytechnique and College de France, Paris, France

The study of the real-time dynamics dynamics of solids perturbed by short laser pulses is an intriguing opportunity of ultrafast materials science. Previous theoretical work on pump-probe photoemission spectroscopy revealed spectroscopic signatures of electron-boson coupling [1, 2], which are reminiscent of features observed in recent pump-probe photoemission experiments on cuprate superconductors [3, 4]. Here we investigate the ordered state of electron-boson mediated superconductors subject to laser driving using Migdal-Eliashberg theory on the Kadanoff-Baym-Keldysh contour. We extract the characteristic time scales on which the non-equilibrium superconductor reacts to the perturbation, and their relation to the coupling boson and the underlying order.

[1] M. Sentef et al., Phys. Rev. X 3, 041033 (2013).
[2] A. F. Kemper et al., Phys. Rev. B 90, 075126 (2014).
[3] J. Graf et al., Nat. Phys. 7, 805 (2011);
W. Zhang et al., Nat. Comm. 5, 4959 (2014).
[4] J. D. Rameau et al., Phys. Rev. B 89, 115115 (2014).

TT 99.5 Thu 16:00 H 2053

Conformal phase transition as a new perspective on conventional superconductors — •Flavio Nogueira[1] and Asle Sudbo[2] — [1]Theoretische Physik III, Ruhr-Universität Bochum — [2]Dept. of Physics, Norwegian University of Science and Technology

We argue that the phase transition in strong type I superconductors features charged fluctuations, meaning that it is essentially driven by thermal fluctuations of the magnetic field. This is simply a consequence of the small value of the Ginzburg parameter in the deep type I regime. We substantiate this conclusion by a generalization of the Ginzburg criterion to include charged fluctuations. Finally, we demonstrate by means of a renormalization group analysis that the correlation length actually does not obey a power law as function of $T - T_c$. Rather it features an essential singularity at T_c, which is characteristic of a so called conformal phase transition, one known example of it being the Berezinski-Kosterliz-Thouless (BKT) phase transition in two-dimensional superfluids. We argue that a similar behavior happens in three-dimensional strongly type I superconductors. One important prediction from our theory that may be tested experimentally by microwave measurement is a universal discontinuous jump in the superfluid density.

TT 99.6 Thu 16:15 H 2053

Surface instability of nodal noncentrosymmetric superconductors — •Carsten Timm[1], Stefan Rex[2], and Philip M. R. Brydon[3] — [1]Institute of Theoretical Physics, Technische Universität Dresden, Germany — [2]Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway — [3]Condensed Matter Theory Center, The University of Maryland, College Park, U.S.A.

It has been proposed that nodal noncentrosymmetric superconductors show flat bands of zero-energy surface states [1,2]. Such surface states would realize a two-dimensional gas of Majorana fermions with interesting properties. However, the proposal was based on the assumption that the superconducting gaps assume constant bulk values even in the presence of a surface. We here employ self-consistent mean-field theory to calculate the gaps and the surface states for a slab of finite thickness. We find two phase transitions upon lowering the temperature: At a higher temperature T_c, the slab becomes superconducting and develops flat surface bands. At a lower temperature T_s, time-reversal invariance is spontaneously broken in the surface region and the surface bands become dispersive and are pushed away from the Fermi energy.

[1] A. P. Schnyder and S. Ryu, Phys. Rev. B **84**, 060504(R) (2011).
[2] P. M. R. Brydon, A. P. Schnyder, and C. Timm,
Phys. Rev. B **84**, 020501(R) (2011).

TT 99.7 Thu 16:30 H 2053

Collective modes in superconductors without inversion symmetry — •Nikolaj Bittner[1], Dietrich Einzel[2], Ludwig Klam[1], and Dirk Manske[1] — [1]Max–Planck–Institut für Festkörperforschung, D–70569 Stuttgart, Germany — [2]Walther–Meißner–Institut für Tieftemperaturforschung, D–85748 Garching, Germany

The collective modes characteristic of conventional and unconventional superconductors include the Anderson–Bogoliubov (or gauge) mode ω_{G} as well as the condensate plasma mode ω_{P}, to which the gauge mode gets shifted as a consequence of the Anderson–Higgs mechanism (AHM). A unique property of non–centrosymmetric superconductors (ncs) is the coexistence of spin–singlet (Δ_s) and triplet (Δ_{tr}) energy gaps. In the limit of strong spin–orbit coupling there arises a two–band (two–gap) structure, which automatically implies the existence of a new massive collective mode ω_{L}, discovered by A. J. Leggett in 1966 for ordinary two–band superconductors, the so–called Leggett mode. In this contribution we focus on the analysis of the electromagnetic response of the superconducting condensate and specify for the first time the collective modes ω_{G}, ω_{P} and ω_{L} in ncs systems of cubic and tetragonal symmetry. Particular emphasis is on the analysis of Leggett's collective mode in ncs systems for which we can show that (i) it is, besides the gauge mode, necessary to guarantee charge conservation, (ii) the AHM only slightly modifies its dispersion and leaves its mass unaffected, (iii) it survives in the limit of vanishing triplet admixture $t = \Delta_{tr}/\Delta_s$ to the singlet energy gap and (iv) its form is symmetry–dependent (cubic, tetragonal) for finite triplet admixture t.

15 min. break.

TT 99.8 Thu 17:00 H 2053

The fate of the superconducting gap close to two magnetic Shiba impurities — •Tobias Meng[1,2], Silas Hoffman[2], Jelena Klinovaja[2], and Daniel Loss[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

As a potential host for Majorana zero energy bound states, chains of magnetic impurities in superconductors are attracting an increasing amount of attention. Working towards a better understanding of the physics of such chains, we address the effect of a single, and of two close magnetic impurities in a superconductor. Specifically, we analytically calculate how the presence of the Cooper pair breaking Shiba impurities locally reduces the superconducting gap. We show that the gap renormalization can favor an antiferromagnetic ordering of the impurities that competes, e.g., with the RKKY exchange.

TT 99.9 Thu 17:15 H 2053

Collective modes in superconducting rhombohedral graphite — •Ville Kauppila[1], Timo Hyart[2], and Tero Heikkilä[2] — [1]O.V. Lounasmaa Laboratory, Aalto University, Finland — [2]University of Jyväskylä, Finland

Recently it was realized that coupling particles with a Dirac dispersion (such as electrons in graphene) can lead to a topologically protected state with flat band dispersion. Such a state could support superconductivity with unusually high critical temperatures[1]. Perhaps the most promising way to realize such coupling in real materials is in the surface of rhombohedrally stacked graphite.

We consider collective excitations (i.e. the Higgs modes) in surface superconducting rhombohedral graphite. We find two amplitude and two phase modes corresponding to the two surfaces of the graphite where the superconductivity lives. We calculate the dispersion of these modes. We also derive the Ginzburg-Landau theory for this material. We show that in superconducting rhombohedral graphite, the collective modes, unlike in conventional BCS superconductors, give a large contribution to thermodynamic properties of the material.

[1] T.T. Heikkila, N.B. Kopnin, G.E. Volovik,
Phys. Rev. B 83, 220503(R) (2011)

TT 99.10 Thu 17:30 H 2053

Interaction effects along the edge of a topological superconductor — •Johannes S Hofmann[1,2], Andreas P Schnyder[2], and Fakher Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Würzburg, Deutschland — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Deutschland

Topological nodal superconductors, such as d_{xy}-wave and nodal noncentrosymmetric superconductors, exhibit protected zero-energy flat-band edge states. These zero-energy edge modes are protected by time-reversal and translation symmetry and their stability is guaranteed by the conservation of a quantized topological invariant. Here, we study the fate of these flat-band edge states in the presence of interactions. We find that Hubbard interactions lead to spontaneous breaking of time-reversal or translation symmetry at the edge of the system. For the d_{xy}-wave superconductor in the presence of attractive Hubbard interactions we find that the flat-band states become unstable towards the formation of a charge-density wave state or a state with s-wave type pairing correlations. Repulsive Hubbard interactions, on the other hand, induce ferromagnetic order at the edge of the d_{xy}-wave superconductor.

TT 99.11 Thu 17:45 H 2053

Superconductivity of heavy fermions in the Kondo lattice model — •Steffen Sykora[1] and Klaus W. Becker[2] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany

Understanding of the origin of superconductivity in strongly correlated electron systems is one of the basic unresolved problems in physics. Examples for such systems are the cuprates and also the heavy-fermion metals, which are compounds with $4f$ and $5f$ electrons. In all these materials the superconducting pairing interaction is often believed to be predominantly mediated by spin fluctuations and not by phonons as in normal metals. For the Kondo-lattice model we present results, which are derived within the Projective Renormalization Method (PRM). Based on a recent study of the one-particle spectral function for the normal state we first derive an effective Hamiltonian which describes heavy fermion quasiparticle bands close to the Fermi surface. An extension to the superconducting phase leads to d-wave solutions for the superconducting order parameter in agreement with recent STM measurements.