TT 22: Superconductivity: Theory

Time: Tuesday 9:30–12:30 Location: H7

TT 22.1 Tue 9:30 H7

Doping induced superconductivity in compressed hydrides, an *ab-initio* investigation — •Antonio Sanna[1] and José A. Flores-Livas[2] — [1]Max Planck Institute of microstructure physics, Halle (Saale), Germany — [2]University of Basel, Department of Physics, Basel, Switzerland

Under pressure hydrides have reached extremely high superconducting critical temperatures rekindling the dream of a room temperature superconductor.

Unfortunately, many (if not most) chemical compounds containing hydrogen only metallize at extreme pressures. A possible solution to this issue could be to use a heavy chemical doping, that can render metallic and even superconducting a semiconducting system.

Following this idea we have investigated, by *ab initio* methods, if doping can be used to obtain high-T_C superconductivity in hydrides. We have considered three examples: H_2O [1], as one of the most abundant, and best studied, hydrides; polyethylene [2] a polymeric hydrocarbon, as representative of the immense family of organic compounds; and the (6,0) graphene nanotube [3] with exohedral hydrogenation.

[1] J.A. Flores-Livas et al., Scientific Reports **7**, 6825 (2017)
[2] J.A. Flores-Livas et al., Eur. Phys. J. B **91** 176(2018)
[3] A. Sanna et al., Eur. Phys. J. B **91** 177 (2018)

TT 22.2 Tue 9:45 H7

Investigating the effect of impurities on the superconducting state — •Tom Saunderson[1], Gábor Csire[2], James Annett[1], Balázs Úfalussy[2], and Martin Gradhand[1] — [1]HH Wills Laboratory, University of Bristol, UK — [2]Wigner Research Centre for Physics, PO Box 49, H-1525 Budapest, Hungary

Our understanding of the superconducting state in real materials is still very limited. Not only are the driving mechanisms for many unconventional superconductors poorly understood but also the coupling to magnetic layers or the effect of impurities represent major conceptual challenges [1]. Furthermore, the effects of interfaces, impurities and spin orbit coupling on spin dependent transport, properties well established in the normal state, attract more and more interest [2]. Here we present the implementation of the Bogoliuobov-de Gennes (BdG) equation into a Green′s function (KKR) first principles method [3]. Due to it being a Green′s function method, it is possible to model bulk materials including impurities and interfaces without the need of artificial supercells. We parameterise the pairing potential but solve the BdG equation self-consistently incorporating the microscopic properties of real materials. Here we are going to present calculations for various test cases of simple superconductors and will investigate the influence of impurities on the superconducting state with a particular future interest in the influence of magnetic impurities.

[1] G. R. Stewart, Adv. in Phys., **66**, 75 (2017)
[2] M. Eschrig, Rep. Prog. Phys,, **78**, 104501 (2015)
[3] G. Csire *et al*, Phys. Rev. B,, **91**, 165142 (2015)

TT 22.3 Tue 10:00 H7

Reduced Density Matrix Functional Theory for Superconductors — Jonathan Schmidt, •Carlos Benavides Riveros, and Miguel Marques — Martin-Luther Universität Halle Wittenberg

We present a new ab-initio theory for superconducting systems with nonlocal external potentials based on the one-particle reduced density matrix $\rho(r, r')$, the anomalous density $\chi(r, r')$ and the nuclear density $D(r, r')$. We prove that all the system's equilibrium properties are determined uniquely by these three quantities and deduce a variational principle for the grand canonical potential in terms of them. By replacing the local electronic density, which is used in density functional theory for superconductors (SC-DFT), with the non-local one-particle reduced density matrix, our theory is able to solve difficulties which arise in SC-DFT through the combination of local and non-local quantities.

Analogue to the Kohn-Sham system in DFT, we prove the existence of a Kohn-Sham system that is able to reproduce ρ, χ and D of an interacting system at finite temperature. On the basis of the Kohn-Sham system, we obtain a set of Bogoliubov-De Gennes-like single particle equations. Finally, we derive a first exchange-correlation functional through the Sham-Schlüter connection.

TT 22.4 Tue 10:15 H7

Feasible model for light-induced interband pairing — Sergio Porta[1,2], •Lorenzo Privitera[2], Niccolò Traverso Ziani[1,2], Fabio Cavaliere[1], and Björn Trauzettel[2] — [1]Dipartimento di Fisica, Università di Genova, 16146 Genova, Italy — [2]Institute of Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

Recent theoretical works [1,2] have highlighted the existence of a purely electronic mechanism for the appearance of non-equilibrium superconductivity in a resonantly driven semiconductor with repulsive interband interactions. The original proposals relied anyway on the existence of a specific fermionic dissipation mechanism and the careful simultaneous tailoring of the electronic dispersion relation and the electron-electron interaction.

In this work we show that this mechanism is actually more general and does not need any special tuning of the parameters. When considering a pair of bands with the same sign of concavity, we indeed demonstrate that interband pairing emerges under the natural assumptions of the presence of phononic baths and radiative recombination. In light of these findings, we show how the appearance of superconductivity can be understood in terms of standard equilibrium interband BCS theory. Finally, we conclude by presenting a phase diagram for the steady state of the model.

[1] G. Goldstein, C. Aron, and C. Chamon, Phys. Rev. B 91, 054517 (2015)
[2] O. Hart, G. Goldstein, C. Chamon and C. Castelnovo, arXiv:1810.12309

TT 22.5 Tue 10:30 H7

Higgs spectroscopy for periodically driven unconventional superconductors — •Lukas Schwarz and Dirk Manske — Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

Higgs spectroscopy for superconductors in nonequilibrium is a new method to obtain phase-sensitive information about the underlying gap symmetry [1]. One experimental setup to observe the Higgs mode is third-harmonic generation (THG), where the driving frequency of a multicycle THz pulse is brought in resonance with the Higgs mode. This was already successfully demonstrated for s-wave superconductors [2]. We show that THG can be used to observe also additional Higgs modes predicted to occur in d-wave superconductors [3]. They show up as a second resonance in the THG response. Such an additional resonance was found in recent THG experiments on cuprates and can be explained by our theory [4]. This theory is not limited to d-wave superconductors but applies in general to any gap symmetry where multiple Higgs modes are possible. Thus, THG experiments extend the repertoire of Higgs spectroscopy experiments and can be used for the identification of gap symmetries of unconventional superconductors.

[1] B. Fauseweh et al., arXiv:1712.07989 (2017)
[2] R. Matsunaga et al., Science 345, 1145 (2014)
[3] L. Schwarz et al., Higgs spectroscopy for periodically driven unconventional superconductors, arXiv
[4] H. Chu et al., New collective mode in superconducting cuprates uncovered by Higgs spectroscopy, arXiv

15 min. break.

TT 22.6 Tue 11:00 H7

Hall coefficient in two-dimensional metals with spiral magnetic order and application to cuprate high-T_c superconductors — •Johannes Mitscherling and Walter Metzner — Max Planck Institute for Solid State Research, Stuttgart, Germany

Charge transport measurements in high magnetic fields recently shed new light on the non-superconducting ground state in cuprate high-T_c superconductors [1]. In particular, Hall measurements yield a drop of the Hall number indicating a phase transition associated with a Fermi surface reconstruction. On the theoretical side, spiral magnetic order (or quasi-order) remains a hot candidate for the Fermi surface reconstruction mechanism. The electromagnetic response of spiral magnetic states has already been analyzed for small relaxation rates [2]. However, the relaxation rate in the cuprate samples studied experimentally

is sizable. We have, thus, derived, for the first time, a complete formula (including all interband contributions) for the Hall conductivity in the low field limit $\omega_c\tau \ll 1$ [3]. We use the complete expressions to study the importance of a sizable relaxation rate and show that the observed Hall number drop in cuprates can be fitted with realistic parameters.

[1] Badoux *et al.*, Nature **531**, 210 (2016)
[2] Voruganti *et al.*, PRB **45**, 13945 (1992)
[3] Mitscherling and Metzner, PRB **98**, 195126 (2018)

TT 22.7 Tue 11:15 H7

Unconventional superconductivity in the 2D Hubbard model: weak-coupling renormalization group — •Sebastian Wolf[1], Thomas Schmidt[2], and Stephan Rachel[1] — [1]School of Physics, University of Melbourne, Parkville, VIC 3010, Australia — [2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511, Luxembourg

We employ the weak-coupling renormalization group approach to study unconventional superconducting phases emerging in the extended, repulsive Hubbard model on paradigmatic two-dimensional lattices. Repulsive interactions usually lead to higher-angular momentum Cooper pairing. By considering not only longer-ranged hoppings, but also nonlocal electron-electron interactions, we are able to find superconducting solutions for all irreducible representations on the square and hexagonal lattices, including extended regions of chiral topological superconductivity. For paradigmatic 2D lattices, we provide detailed superconducting phase diagrams as well as the coupling strengths which quantify the corresponding critical temperatures depending on the bandstructure parameters, band filling, and interaction parameters.

TT 22.8 Tue 11:30 H7

Kohn-Luttinger superconductivity and chirality in twisted bilayer graphene — •Tobias Stauber[1], Jose Gonzalez[2], Tony Low[3], and Guillermo Gomez-Santos[4] — [1]Departamento de Teoria y Simulacion de Materiales, Instituto de Ciencia de Materiales de Madrid, CSIC, E-28049 Madrid, Spain — [2]Instituto de Estructura de la Materia, CSIC, E-28006 Madrid, Spain — [3]Department of Electrical & Computer Engineering, University of Minnesota, Minneapolis, Minnesota 55455, USA — [4]Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Twisted bilayer graphene has attracted much attention due to its novel electronic and optical properties. Here, we will present our recent theoretical results on the superconducting instability and also on the inherent chirality of the system. In particular, we will show that the Kohn-Luttinger mechanism might be active in TBL [1]. Furthermore, we find a paramagnetic response around the neutrality point, a longitudinal Hall effect and longitudinal plasmonic excitations which are accommodated by a longitudinal magnetic moment [2,3].

[1] J. Gónzalez and T. Stauber, arXiv:1807.01275
[2] T. Stauber, T. Low, and G. Gómez-Santos, Phys. Rev. Lett. 120, 046801 (2018)
[3] T. Stauber, T. Low, and G. Gómez-Santos, Phys. Rev. B 98, 195414 (2018)

TT 22.9 Tue 11:45 H7

Analytic study of dissipative phase transitions in a driven nonlinear resonator model — •Mikhail Pletyukhov — RWTH Aachen University, Institute for Theory of Statistical Physics, 52074 Aachen, Germany

The Kerr nonlinearity model plays an important role in circuit QED. At strong microwave drive and weak nonlinearity it is known to feature a bistable behavior, which can be interpreted as a dissipative phase transition. In this talk, I show on the basis of the analytical solution for the steady state of this model that some effective limiting procedure (mimicking the thermodynamic limit) does lead to a jump in observables - the property of the first order transition, and I give a full analytic charaterization of this transition. In the two-photon driven Kerr model, a similar consideration allows one to characterize a second-order transition occurring in it, and this issue is also addressed in the talk.

Invited Talk TT 22.10 Tue 12:00 H7

Superconducting films and interfaces: Novel features from spin imbalance and Rashba spin-orbit coupling — •Gertrud Zwicknagl — Institut f. Mathemat. Physik, TU Braunschweig, Braunschweig, Germany

In recent years, the manufacturing of controlled ultra-thin superconducting films has made impressive progress.Important examples are monoatomic or monomolecular layers on a substrate, superconducting layers in a superlattice, or superconducting interfaces and surfaces. These systems have in common the absence of inversion symmetry and hence the presence of Rashba-type spin-orbit energy λ. The latter can be modified to some extent by varying the thickness, the number of layers, or by applying an electric voltage. The subtle interplay of spin imbalance created by a magnetic field and the Rashba spin-orbit interaction gives rise to novel phenomena in quasi-2D superconductors which, in turn, could provide new functionalities. I discuss the results of a microscopic theory of superconducting films with population imbalance which are subject to Rashba spin- orbit interaction. The full range from small to large spin-orbit interaction is covered. A quantum phase transition at a critical value of the spin-orbit energy λ_c is predicted where abrupt changes in the superconducting state are expected. It is tempting to speculate, that this feature might give rise to novel phenomena. For example, the Josephson interference effects should change dramatically near this point. These and other open issues together with recent work and promising future directions will be discussed.