TT 39: Superconductivity: (General) Theory

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

TT 39.1 Wed 9:30 HSZ 103

Induced Superconductivity in the Hubbard model — •Nikolaj Bittner[1], Takami Tohyama[2], and Dirk Manske[1] — [1]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]Department of Applied Physics, Tokyo University of Science, Tokyo 125-8585, Japan

Recent development of optical pulses at THz and mid-infrared frequencies has reported indications of photo-induced superconductivity at temperatures much higher than superconducting transition temperature (Tc) in cuprate superconductors [1] and K-dopes C_{60} [2]. These are now a hot topic in the field of superconductivity.

In this contribution we present a theoretical study of the nonequilibrium dynamics in the one-dimensional extended Hubbard model at half filling. Particular emphasizes is on the possibility to induce superconductivity in this system driven out of equilibrium. Within the framework of the time-dependent Lanczos algorithm the time evolution of the Hubbard model is investigated for two different nonequilibrium scenarios, which occur by (i) an interaction quench and by (ii) action of a light pulse. For both cases the time dependent optical conductivity and the superconducting correlation functions are calculated. In particular, it was observed from these calculations appearance of a transient Meissner effect, which is a fingerprint of the induced superconductivity. This is in agreement with the obtained correlation functions and opens a new way to induce superconductivity in an experiment.

[1] S. Kaiser et al. PRB, 89, 184516 (2014);
D. Fausti et al. Science 331, 189 (2011)
[2] M. Mitrano et al. Nature, 530, 461 (2016)

TT 39.2 Wed 9:45 HSZ 103

Plaquette valence bond theory of high-temperature superconductivity — •Malte Harland[1], Mikhail I. Katsnelson[2], and Alexander I. Lichtenstein[3] — [1]Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany — [2]Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525AJ Nijmegen, The Netherlands — [3]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, Hamburg 22761, Germany and Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany

We present a strong-coupling approach to the theory of high-temperature superconductivity based on the observation of a quantum critical point in the plaquette within the t, t' Hubbard model. The crossing of ground state energies in the $N = 2, 3, 4$ sectors occurs for parameters close to the optimal doping. The theory predicts the maximum of the $d_{x^2-y^2}$-wave order parameter at the border between localized and itinerant electron behavior and gives a natural explanation for the pseudo-gap formation via soft-fermion mode related to local singlet states of the plaquette in the environment. Our approach follows the general line of resonating valence bond theory stressing a crucial role of singlets in the physics of high-T_c superconductors, but focuses on the formation of *local* singlets.

TT 39.3 Wed 10:00 HSZ 103

The T-dependence of the scattering rate in cuprates: Insights from diagrammatic extensions of DMFT — •Marie-Therese Philipp[1,2], Georg Rohringer[2], Clemens Watzenböck[1], Thomas Schäfer[1], Hartmut Hafermann[3], Jan M. Tomczak[1], Karsten Held[1], Alexey Rubtsov[2], and Alessandro Toschi[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Russian Quantum Center, Novaya street, 100, Skolkovo, Moscow region 143025, Russia — [3]Mathematical and Algorithmic Sciences Lab, France Research Center, Huawei Technologies Co. Ltd., 92100 Boulogne-Billancourt, France

We analyze here some of the most recent experimental results[1] for the resistivity ρ and the Hall-resistivity ρ_H of the high-T_c superconducting cuprates. Surprisingly, the measured ratio ρ/ρ_H shows a universal, Fermi-liquid (FL) temperature dependence across the whole phase diagram. In the simplest Drude picture, this ratio would correspond to FL scattering rate ($\gamma \propto T^2$). In this context, γ can be computed in many-body theory from the imaginary part of the self-energy at the Fermi surface $[-Im(\Sigma(w = 0, k_F))]$. In particular, to estimate $-Im(\Sigma(w = 0, k_F))$, we have employed diagrammatic extensions of DMFT, namely the dual fermion (DF) approach and the dynamical vertex approximation (DΓA). The obtained temperature dependences will be compared to a more precise, but also challenging, direct estimate of ρ/ρ_H, by means of the *bubble-like* term of the corresponding conductivity tensors.

[1] N. Barišić, et al. (2015) arXiv:1507.07885

TT 39.4 Wed 10:15 HSZ 103

Charge and current orders in the cuprates: implications from spin-fermion model with overlapping hot spots. — •Pavel A. Volkov and Konstantin B. Efetov — Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Experiments carried over the last years on the underdoped cuprates suggest the presence of a variety of symmetry-breaking phenomena in the pseudogap phase. Charge-density waves, breaking of C_4 rotational symmetry, as well as time-reversal symmetry breaking have all been observed in several cuprate families. Unification of these phenomena thus poses a crucial theoretical challenge. We address this issue in the framework of the spin fluctuation scenario, where the low-energy fermions interact through the exchange of antiferromagnetic fluctuation quanta, paramagnons. We study particle-hole instabilities in a model explicitly taking into account two regions of the Fermi surface: around $(0, \pi)$ and $(\pi, 0)$. For a quasi-1D dispersion in both regions, we show that for sufficiently small $|\varepsilon(\pi, 0) - E_F|$, the leading instability is a d-form factor Fermi surface deformation (Pomeranchuk instability). It naturally produces a C_4-breaking and supports the formation of a unidirectional bond-oriented d-form factor CDW at lower temperatures, consistent with experiments. Additionally, we show that the Fermi surface curvature in the antinodal regions promotes a state formed by current loops organized in an antiferromagnetic structure (as in the d-density wave state), and thus breaking time-reversal symmetry.

TT 39.5 Wed 10:30 HSZ 103

Three-band superconductors with broken time reversal symmetry ground states — •Yuriy Yerin[1,2], Alexander Omelyanchouk[2], Stefan-Ludwig Drechsler[3], Jeroen van den Brink[3], and Dmitri Efremov[3] — [1]Institute for Physics of Microstructures, Russia — [2]Institute for Low-Temperature Physics , Ukraine — [3]Institute for Theoretical Solid State Physics, Leibnitz Institute IFW-Dresden, Germany

Within the Ginzburg-Landau formalism we provide a classification of all possible ground states of a three-band superconductor (SC) where either states with broken time-reversal symmetry (BTRS) or a single non-BTRS ground state of s-wave symmetry are realized. We track possible evolutions of the BTRS ground state in an external magnetic field. We show that an external magnetic field may trigger transitions between BTRS and non-BTRS states. We propose to use the current induced magnetic flux response of samples with a doubly-connected geometry as a suitable experimental searching method for the detection of BTRS ground states as well as of corresponding metastable excited state in three-band SC. The latter can be involved in a flux regime nonadiabatically switched on. Due to frustration of the three-band order parameter components topological solitons and other inhomogeneous topological states are possible and will be briefly discussed, too.

TT 39.6 Wed 10:45 HSZ 103

f-wave triplet superconductivity in a twisted triangular Hubbard tube as a model of $A_2Cr_3As_3$ — Sahinur Reja[1] and •Satoshi Nishimoto[2,3] — [1]Indiana University, Bloomington, USA — [2]TU Dresden, Germany — [3]IFW Dresden, Germany

Triplet superconductivity (SC) recently has been one of the active research topics partly due to its intrinsic connection to quantum computations. In this contex, we study the ground state properties of a twisted triangular Hubbard tube using the perturbation theory and density-matrix renormalization group method. We show that two electrons in an odd-site Hubbard ring always form a spin-triplet pair, and subsequently a polarized ferromagnetic (FM) order is stabilized in a wide range of electron filling (n) when these rings are weakly coupled. By calculating the binding energy and spin gap, we confirm the presence of the spin-triplet SC after melting of the FM order with increasing the inter-triangle couplings (t_2). We show that triplet SC

pair correlations are consistent with the f-wave channel. We present a detailed n-t_2 phase diagram which features also singlet SC at $n \sim 1$ and $t_2 \sim 1$. Finally we argue that this model has possible relevance to the f-wave SC observed in alkali chromium arsenides $A_2Cr_3As_3$ (A=K,Rb,Cs).

TT 39.7 Wed 11:00 HSZ 103

Inflated nodes in multiband superconductors with broken time-reversal symmetry — •Carsten Timm[1], Daniel F. Agterberg[2], and Philip M. R. Brydon[3] — [1]Institute of Theoretical Physics, Technische Universität Dresden, Germany — [2]Department of Physics, University of Wisconsin, Milwaukee, U.S.A. — [3]Department of Physics, University of Otago, Dunedin, New Zealand

It is commonly believed that superconductors fall into one of three classes: They can have a full energy gap, a gap with point nodes, or a gap with line nodes. We show that multiband, even-parity, nodal superconducting states that break time-reversal symmetry do not belong to these classes. Instead, they *generically* possess two-dimensional Fermi surfaces. These Fermi surfaces can be visualized as being generated by "inflating" point and line nodes into spheroids and tori, respectively. The inflated nodes are topologically protected by a $\mathbb{Z}_2$ invariant, which we give in terms of a Pfaffian. We also show that such states can be *energetically* stable in spite of the extended Fermi surfaces; they form the state with the lowest free energy if spin-orbit coupling is sufficiently strong.

15 min. break.

TT 39.8 Wed 11:30 HSZ 103

Mutually attracting spin waves in the square-lattice quantum antiferromagnet — •Kai Phillip Schmidt[1], Michael Powalski[2], and Götz S. Uhrig[2] — [1]FAU Erlangen-Nürnberg, Erlangen, Germany — [2]TU Dortmund, Dortmund, Germany

Spin waves (magnons) in two dimensions are the potential glue in high-temperature superconductors so that their quantitative understanding is mandatory. Yet even for the fundamental case of the undoped Heisenberg model on the square lattice a consistent picture is still lacking. Significant spectral continua are taken as evidence of the existence of fractional excitations (spinons), but descriptions in terms of spinons fail to show the established absence of an energy gap. Here a fully consistent picture of the dynamics of magnetism in the square-lattice quantum antiferromagnet is provided which agrees with the experimental findings. The key step is to capture the strong attractive interaction between the spin waves.

TT 39.9 Wed 11:45 HSZ 103

Ab-initio characterization of superconductivity in the elemental phases of phosphorus: from black-P up to 350 GPa — •Antonio Sanna[1], Jose Flores-Livas[2], Gianni Profeta[3], and Lilia Boeri[4] — [1]MPI for Microstucture Physics, Halle, Germany — [2]University of Basel, Switzerland — [3]University of L'Aquila, L'Aquila, Italy — [4]TU Graz, Austria

We present the result of a complete ab-initio characterization of elemental phosphorus in its structural and superconducting properties.

At low pressure we discuss the possibility of superconductivity in Black-P upon doping. In the high pressure regime we investigate thermodynamic stability by performing structural search with the minima hopping method. This way identifying structures that are likely to form upon compression. On the low enthalpy structures we perform full electronic and phononic characterization within DFT-PBE. Superconducting properties are predicted by means of Density Functional Theory for Superconductors.

Apart from several interesting predictions, calculations provide a nice interpretation of the existing experimental data, in particular of the evidence that different experimental procedures lead to significantly different values of the critical temperature.

TT 39.10 Wed 12:00 HSZ 103

First principles based proximity effect of superconductor-normal metal heterostructures — •Gabor Csire[1], Balazs Ujfalussy[1], and Jozsef Cserti[2] — [1]Wigner RCP, Budapest, Hungary — [2]Eotvos University, Budapest, Hungaty

We investigate the proximity effect in superconductor-normal metal heterostructures based on first principles calculations with treating the pairing potential as an adjustable parameter. The superconducting order parameter (anomalous density) is obtained from the Green-function by solving the Kohn-Sham-Bogoliubov-de Gennes equations with the Screened Korringa-Kohn-Rostoker method. The results are interpreted for an Au/Nb(001) system. The layer resolved anomalous spectral function is also obtained which is closely related to the superconducting order parameter. We show that the proximity effect can be understood via the anomalous spectral function.

TT 39.11 Wed 12:15 HSZ 103

Friedel-oscillations in inhomogeneous topological superconductors — •Lars Lauke[1], Mathias Scheurer[1], Andreas Poenicke[1,2], and Jörg Schmalian[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Deutschland — [2]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

In order to investigate Majorana bound states in p-wave superconductors and to reveal the precise influence of boundaries and inhomogeneities on the local structure of competing superconducting order parameters, we solve inhomogeneous Bogoliubov-de Gennes equations. Going beyond the quasi-classical approach we examine in particular the role of Friedel-oscillations due to inhomogeneities and the surface of the superconductor and analyse the distinct behaviour of the p-wave and the surface induced s-wave pairing amplitudes.

TT 39.12 Wed 12:30 HSZ 103

Exotic vortex configurations and superconductors with shallow bands — •Sebastian Wolf[1], Alexei Vagov[1], Arkady Shanenko[2], José Albino Aguiar[2], and Vollrath Martin Axt[1] — [1]Institut for Theoretical Physics III, University Bayreuth, Germany — [2]Departamento de Física, Universidade Federal de Pernambuco, Recife, Brazil

Experiments revealed that the magnetic response of superconducting materials that are close to the interchange between type I and type II may be very different from either of the two standard types [1,2]. The interval of such non-conventional behavior, referred to as the inter-type superconductivity, is rather small in traditional materials but can be considerably enlarged in non-conventional multi-band superconductors such as in MgB_2 [2]. Theoretical description of this interval requires an approach beyond the traditional Ginzburg-Landau theory. In our work we investigate inter-type superconductors within the framework of the extended Ginzburg-Landau theory [3].

Using this approach we demonstrated a general enlargement tendency for the inter-type domain in multi-band superconductors, especially when one of the contributing bands is shallow. In order to explain the appearance of non-conventional mixed states we studied details of the vortex-vortex interaction, in particular the crossover between the monotonic and the non-monotonic interaction.

[1] U. Krägeloh, Physics Letters A **28**, 657-658 (1969)
[2] V. Moshchalkov et al., Phys. Rev. Lett. **102**, 117001 (2009)
[3] A. V. Vagov et al., Phys. Rev. B **85**, 014502 (2012)

TT 39.13 Wed 12:45 HSZ 103

Exploring the Efimov effect in conventional superconductors — •Ali Sanayei[1], Pascal Naidon[2], and Ludwig Mathey[1] — [1]Center for Optical Quantum Technologies, Institute for Laser Physics, University of Hamburg, Luruper Chaussee 149, D-22761 Hamburg — [2]RIKEN Nishina Centre, RIKEN, Wako 351-0198, Japan

In this work, we explore the emergence of the Efimov effect in solid state physics. We consider a three-electron system in distinguishable states of (band 1, up), (band 2, up), and (band 2, down) in a solid. The electron in band 1 is located in an otherwise empty band and interacts through a spin-independent interaction with the two up- and down-electrons in band 2, both of which are immersed in a Fermi sea. Introducing a proper renormalization of the coupling constants, we derive a system of two coupled integral equations describing a three-electron eigenstate in momentum space. These equations support a trimer state solution of electrons, which is a demonstration of the Efimov effect in conventional superconductors.

TT 39.14 Wed 13:00 HSZ 103

Multi-particle instability in an imbalanced electron gas — •Gareth Conduit and Thomas Whitehead — Department of Physics, University of Cambridge, UK

We show that in an imbalanced electron gas weak attractive interactions induce a multi-particle instability, binding multiple electrons together. The maximum binding energy per particle is achieved where the ratio of the number of up/down spin particles in the instability is

equal to the ratio of the up/down spin density of states. We use this instability to propose a new superconducting ground state that has lower energy than the FFLO state.