TT 91: Superconductivity: (General) Theory 1

Time: Thursday 11:30–13:00 Location: H 2053

TT 91.1 Thu 11:30 H 2053

***Ab initio* study of the interplay between superconductivity and magnetic fields in MgB_2** — •Alexandros Aperis, Pablo Maldonado, and Peter M. Oppeneer — Uppsala University, Uppsala, Sweden

Among the bulk superconductors broadly accepted to be mediated by phonons, MgB_2 exhibits a record high critical temperature of $T_c = 39$ K. The relatively simple crystal structure of this material makes it an ideal platform to investigate fundamental phenomena, such as the interplay between superconductivity and the Zeeman effect, at the *ab initio* level. Here we combine DFT calculations providing electronic band and phonon dispersions with numerical solutions of the fully anisotropic Eliashberg equations, to provide a complete picture of the modification of the two-band superconductivity in this compound at finite external magnetic fields and temperature. We predict interesting signatures in the $H - T$ phase diagram which could be experimentally probed.

TT 91.2 Thu 11:45 H 2053

Superconductivity in Metal-intercalated Dodecaborides — •Lilia Boeri[1] and Matteo Calandra[2] — [1]ITP-CP TU Graz, Petersgasse 16, 8010 Graz (Austria) — [2]IMPMC, UMR CNRS 7590, Sorbonne Universités - UPMC Univ. Paris 06, MNHN, IRD, 4 Place Jussieu, F-75005 Paris, France

Metal-Intercalated dodecaborides (MB_{12}) display different low-temperature behaviour depending on the nature of the metal atom M [1]. In this work, we employ a method based on real-space (Wannier) interpolation of phonon and electronic wave functions [2], to study from first-principles the fully anisotropic Migdal-Eliashberg of compounds with M=Zr, Sc and Lu, which are superconducting with critical temperatures of 5.82 , 0.39 and 0.48 K respectively. These compounds have long been conventional considered BCS-like superconductors, but recent recent optical and ARPES experiments displayed several anomalies, which were attributed to the presence of localized phonon modes and possible strong correlation effects [3,4].

[1] B.T. Matthias et al., Science **159**, 530 (1968).
[2] M. Calandra, G. Profeta, and F. Mauri,
Phys. Rev. B **82**, 165111 (2010).
[3] S. Thakur et al., Scientific Reports **3**, 3342 (2013).
[4] J. Teyssier et al., Phys. Rev. B **75**, 134503 (2007).

TT 91.3 Thu 12:00 H 2053

Charge Order in Cuprate Superconductors — •Sinan Bulut[1], Arno P. Kampf[1], and Bill A. Atkinson[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Department of Physics and Astronomy, Trent University, Peterborough Ontario, Canada

Motivated by widespread experimental evidence of charge orders in underdoped cuprate superconductors, we study a three band model of a cuprate plane. Our calculations start from a pseudogap-like normal system with a reconstructed Fermi surface, and we search for charge instabilities. From the charge susceptibilities, we identify a charge ordering instability with an ordering wavevector, $\mathbf{q}^*$, that matches experimental results not only with respect to the doping dependence but more importantly regarding its magnitude and direction. Namely, $\mathbf{q}^*$ points *along the Brillouin zone axes*. Thus, our results clarify the discrepancy between many recent theoretical calculations and the experiments. We extend this calculation towards possible loop current instabilities and the charge ordering pattern in bilayer systems.

TT 91.4 Thu 12:15 H 2053

Resonant inelastic X-ray scattering of high-T_C cuprates — •Yi Lu[1] and Maurits W. Haverkort[2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]Max Planck Institute for Chemical Physics of Solids, Dresden

We present a systematic study of resonant inelastic X-ray scattering (RIXS) of high-T_c superconducting cuprates using a single-band model. We show how the RIXS spectra evolve in metals, correlated metals and Mott insulators in the framework of dynamical mean-field theory using a recently developed impurity solver. In light of recent experiments, the dependence of RIXS cross-section on doping and incident photon energy were specifically investigated. Our work clarifies the debated interpretation of RIXS as a measurement of magnetic collective mode or simply incoherent excitations of the particle-hole continuum.

TT 91.5 Thu 12:30 H 2053

Critical analysis of the preformed pair physics: the attractive Hubbard model under a paring forcing field — •Agnese Tagliavini[1], Massimo Capone[2], and Alessandro Toschi[1] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Wien, Austria — [2]Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy

The nature of the pseudogap features observed in correlated materials and its relation with superconductivity is still controversially debated. From the theoretical point of view, a new insight on the underlying physics can be obtained by studying the superconducting response to an external pairing field.

To this aim we consider the attractive Hubbard model where a preformed pair physics is realized in the strong-coupling limit: By means of Dynamical Mean-Field Theory, we study the superconducting response of the model to a static external pairing field (both uniform and local) focusing on the energetics.

We also compare our results with those obtained in the 2D repulsive Hubbard model, which is usually considered the basic model for high-Tc superconductors, where studies with cluster extensions of Dynamical Mean-Field Theory indicate the lack of preformed pairs.

TT 91.6 Thu 12:45 H 2053

Asymmetric Bethe-Salpeter equation for pairing and condensation — •Klaus Morawetz[1,2,3] and Pavel Lipavsky[4] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics (IIP)Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

The Martin-Schwinger hierarchy of correlations is reexamined to derive the recently proposed asymmetric Bethe-Salpeter equation avoiding unphysical repeated collisions. Exceeding the parquet approximation an asymmetry appears in the selfconsistent propagators. This form is superior over the symmetric selfconsistent one since it provides the Nambu-Gorkov equations and gap equation for fermions and the Beliaev equations for bosons without the use of anomalous propagators. The T-matrix with multiple scattering corrections allows to describe superconductivity above and below the critical temperature by the same theoretical footing and provides e.g. a critical velocity of pair excitation larger than the critical velocity of pair breaking in agreement with the experiments.

[1] B. Sopik, P. Lipavský, M. Männel, K. Morawetz, P. Matlock,
Phys. Rev. B 84 (2011) 094529.
[2] K. Morawetz, J. Stat. Phys. 143 (2011) 482-500.
[3] P. Lipavský, K. Morawetz, B. Sopik, M. Männel,
Eur. Phys. J. B 87 (2013) 8-1-10.