0.1 Report on Workshop: Superconductivity 100 Years Later: A Computational Approach

P l a c e: Hotel Porto Conte, Alghero, Sardinia, Italy

D a t e: September 15, 2011 to September 18, 2011

S p o n s o r s: CECAM, Psi-k, ESF-Intelbiomat, Regione Sardegna

O r g a n i z e r s: Lilia Boeri (Max Planck Institute for Solid State Research, Stuttgart, Germany), Sandro Massidda (University of Cagliari, Italy), E.K.U. Gross (Max Planck Institute of Microstructure Physics, Halle, Germany)

Web Page: http://www.fkf.mpg.de/conf/sc100/

Report: The workshop has been scientifically quite successful, the talks have been very interesting with many questions to all the speakers. Both at the round table and during the pauses of the scientific program there have been many discussions on the physics of superconducting materials and on the state-of-the-art and future of the field. Furthermore, all the participant have enjoyed the stimulating and friendly atmosphere of the meeting.

More in detail, the materials under attention have been mostly the pnictides, but also C-related materials as picene, graphene and intercalation graphite compounds, MgB_2, cuprates and ruthenates. For pnictides there has been a wide consensus on the magnetic origin of the superconducting mechanism. The major topics examined in these materials were: (i) the symmetry of the order parameter (Gonnelli, Singh, Mazin, Johannes), with a few experimental presentations (*e.g.* point-contact Andreev reflection spectroscopy, Gonnelli) and the corresponding implications on the nature of the pairing and on the strength of the pairing and electronic interactions; (ii) the nature of magnetism, the spin-fluctuation spectra and the relationship between magnetism and superconductivity (Antropov, Singh, Mazin, Johannes, Toschi); (iii) the importance of correlation effects (Cappelluti, Toschi, and the experimental presentation of the ARPES results by Borisenko); (iii) the role of impurities (Golubov); (iv) multiband effects within an Eliashberg approach (Golubov and Efremov, who substituted Dolgov). (v) the role of the quantum critical point (Mackenzie), renormalization group techniques (Honerkamp). (vi) Optical spectra and correlation effects (Cappelluti).

The talks on cuprates and ruthenates (*e.g.* J. Annet,) were also concerned with the problems of symmetry of the order parameter, magnetism and superconductivity and correlation. The problem of correlation has also been examined in the context of dynamical properties, within the DFT+U approach (Floris).

A significant part of the meeting has been devoted to electron-phonon superconductivity (EPS). Particular attention has been devoted to C-based materials and MgB_2 (Profeta, Yildirim, Calandra), to relativistic effects in Pb (Heid) ,and to experimental techniques to estimate the electron-phonon coupling (Carbone). Always within EPS, we mention the presentation of Sanna

on the status of the density functional theory applied to the superconducting state (SCDFT). Sanna has shown how from the solution of the Sham–Schlüter equations it is possible to derive the Kohn-Sham superconducting gap, and finally obtain a critical temperature which follows very closely the Eliashberg result in the ideal test case where Coulomb interaction is turned off. Finally, we mention two presentations (Bianconi and Peeters) where quantum effects become important at the nanoscale level.

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Superconductivity 100 years later: A computational Approach

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Hotel Porto Conte, Alghero
15-18 September 2011

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Workshop organizers:

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Program

Friday, 16th September 2011

8:50:9:00		Opening remarks
9:00-9:30	**O. K. Andersen**	Speculations about making nickelate high-temperature superconductors
9:30-10:00	**C. Honerkamp**	Unconventional superconductivity viewed by the functional renormalization group – recent applications
10:00-10:30	**F. Carbone**	The electron-phonon coupling in strongly correlated solids studied by ultrafast techniques
10:30-11:00		*Coffee Break*
11:00-11:30	**A. Bianconi**	Shape resonances in multigap superconductors: a common pairing mechanism in pnictides, diborides and cuprates
11:30-12:00	**V.P. Antropov**	Spin-fluctuations induced metallicity, and key magnetic interactions in super-conducting iron pnictides and selenides
12:00-12:30	**S. Borisenko**	Superconductivity and magnetism in iron pnictides
12:30-14:30		*Lunch Break*
14:30-15:00	**R. S. Gonnelli**	Directional point-contact Andreev-reflection spectroscopy of Fe-based superconductors: Gap symmetry and Fermi surface topology
15:00-15:30	**O. V. Dolgov**	Multiband Eliashberg Model for Pnictides
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17:00-20:00		*Poster Session*
20:00		*Dinner*

Saturday, 17th September 2011

9:00-9:30	**D. J. Singh**	Superconductors Near Magnetism
9:30-10:00	**A. Mackenzie**	Phase formation in quantum critical systems
10:00-10:30	**J. Annett**	Intrinsic orbital magnetism and optical dichroism of the multi-band pairing state of the chiral superconductor Sr2RuO4
10:30-11:00		*Coffee Break*
11:00-11:30	**G. Profeta**	How to make graphene superconducting
11:30-12:00	**A. Floris**	Vibrational properties of MnO and NiO from DFT+U-based Density Functional Perturbation Theory
12:00-12:30	**A. Sanna**	State of the art and new developments in superconducting density functional theory
12:30-14:30		*Lunch Break*
14:30-15:00	**R. Heid**	Electron-phonon coupling and superconductivity in bulk and thin films of lead: importance of relativistic corrections
15:00-15:30	**T. Yildirim**	Electron-Phonon Coupling From Finite-Displacement Approach: A Case Study for Metal Doped Picene and Fe-based Superconductors
15:30-16:00	**M. Calandra**	Adiabatic and non-adiabatic phonon frequencies in a Wannier function approach:applications to CaC6, MgB2 and K-doped Picene
16:00-17:30		*Round Table*
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Sunday, 18th September 2011

9:00-9:30	**I. I. Mazin**	Symmetry-allowed pairing states in overdoped 122 iron selenides
9:30-10:00	**E. Cappelluti**	Interband interactions and optical conductivity in iron-based superconductors
10:00-10:30	**F. Peeters**	Quantum size effects in nano-scale superconductors
10:30-11:00		*Coffee Break*
11:00-11:30	**M. Johannes**	Magnetism, superconductivity and spin fluctuations in Fe-based superconductors
11:30-12:00	**A. A. Golubov**	Strong impurity scattering in multiband superconductors
12:00-12:30	**A. Toschi**	Spectral and magnetic properties of the iron-based superconductors: The role of electronic correlations
12.30-12.50		Closing remarks
13:00-14:30		*Lunch Break*
14:30-19:00		*Excursion*

Invited Talks

Speculations about making nickelate high-temperature superconductors.

Xiaoping Yang[1], O. K. Andersen[1], P. Hansmann[2], A. Toschi[2], K. Held[2]

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To my knowledge, no new class of superconductors has been discovered by design, but by chance or by following empirical rules which the next discovery then showed to be of limited validity. The discoveries of the A15 compounds in the seventies, the cuprates in the eighties, MgB_2 in 2001, and the iron pnictides and chalcogenides in 2008 are all examples of this. Despite 25 years' intensive research, high-temperature superconductivity in the cuprates has not been understood, and no superconductor with T_c higher than 150 K has been found since 1993. Even in cases where the mechanism behind the superconductivity has been understood, as for MgB_2, this has so far not helped in designing any better superconductor.

With the new possibilities for building oxide heterostructures, it has been speculated that $d^7 = e_g^1 = (3z^2\text{-}1, x^2\text{-}y^2)^1$ nickelates might be used instead of $d^9 = e_g^3 = (3z^2\text{-}1)^2\ (x^2\text{-}y^2)^1$ cuprates to obtain even higher T_c by confining a single layer of $LaNiO_3$ between layers of an insulating oxide. By using density-functional calculations followed by downfolding to a correlated, low-energy Hubbard Hamiltonian, and solving the latter in the dynamical mean-field approximation (DMFT), we have shown that it might be possible to empty the $(3z^2\text{-}1)$-like band and enforce a single $(x^2\text{-}y^2)$-like conduction band with a Fermi-surface whose shape is like that of the cuprates with the highest T_c [1]. The electronic correlations help to achieve this, but we find that it is even more important to limit the nickelate to a single layer and to choose the confining material properly, i.e. by *cation control*. This also seems to be the way to suppress competing phases with charge and/or spin order, e.g. $2d^7 \rightarrow d^6+d^8$, as our LDA+U calculations show. Experimental studies are under way.[2]

[1] P. Hansmann, Xiaoping Yang, A. Toschi, G. Khaliullin, O. K. Andersen, K. Held; *Phys. Rev. Lett.* **103**, 016401 (2009), *Phys. Rev. B* ***82***, 235123 (2010), Xiaoping Yang et al, *to be published*.

[2] J. W. Freeland,..., J. Chakalian (2011). E Benkiser, ..., B. Keimer *Nature Materials* (2011). A. Boris, ... B. Keimer (2011), M. Ushida,...,Y. Tokura *et al. Phys. Rev. Lett.* **106**, 027001 (2011) .

Intrinsic orbital magnetism and optical dichroism of the multi-band pairing state of the chiral superconductor Sr_2RuO_4.

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The pairing state of the 1.5K superconductor Sr_2RuO_4 is widely believed to be a chiral p-wave spin triplet state of symmetry k_x+ik_y. This is an electronic analogue of the A-phase pairing state of superfluid helium-3. One of the long standing unresolved questions for this superfluid state is the existence or not of an orbital angular momentum $Lz=\hbar$ per Cooper pair, and whether or not this leads to a non-zero macroscopic intrinsic angular momentum of the condensate. For Sr_2RuO_4 the corresponding question is the existence of a non-zero orbital magnetism in the bulk of the material. The existence of such a moment is suggested by muon spin rotation (muSR) measurements and an observation of a non-zero optical Kerr effect below T_c. We present an analysis of both the intrinsic magnetic moment and optical dichroism based upon a multiband chiral pairing state model. We find that the intrinsic Kerr signal is only non-zero in systems with inter-band order parameters related to an interband Josephson-like coupling. This new intrinsic mechanism may explain the Kerr effect observed in strontium ruthenate and possibly other superconductors. We also predict the existence of coherence effects in the temperature dependence of the absorptive part of the ac Hall conductance Im $\sigma_{xy}(\omega, T)$, which can be tested experimentally.

Spin-fluctuations induced metallicity, and key magnetic interactions in superconducting iron pnictides and selenides.

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We analyze the electronic structure and magnetic interactions in $K_2Fe_{4+x}Se_5$ as a function of x. Several common for selenides and pnictides features are found. In particular, the biquadratic coupling is also found important in selenides. However the defect appearance affects the action of biquadratic interactions by creating local distortions which further stabilize nearly ferromagnetic nearest neighbor interactions. We claim that (a) metallic state (which is a prerequisite for superconductivity) can be achieved in $K_2Fe_{4+x}Se_5$ for different values of x and is mainly a result of either a chemical or magnetic disorder among Fe atoms on 'vacancy' sites for x>0. These Fe atoms strongly interact with Fe atoms from the local moment AFM phase observed in insulating $K_2Fe_4Se_4$. Coexistence of these two groups of Fe atoms leads to the formation of two phases. This can be directly related to the coexistence of superconductivity and strong antiferromagnetism observed in K_2FeSe_2 systems. We discuss how such mechanism of the formation of spin fluctuations, can be realized in both families of iron superconductors.

Shape resonances in multigap superconductors: a common pairing mechanism in pnictides, diborides and cuprates.

Antonio Bianconi

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The shape resonance provides a possible mechanism for evading temperature decoherence effects in a quantum condensate [1-4] The shape resonance in the superconducting gaps is basic quantum phenomenon that belong to the class of Fano-resonances or Feshbach-resonances determined by interference between quasi-bound and continuum states introduced by Majorana-Fano-Feshbach. Feshbach resonances are popular in Bose or BCS condensation in ultra-cold gases. In high temperature multiband superconductors shape resonances provide an exchange pairing mechanism that coexists with electron-phonon mechanisms. The shape resonance mechanism for the amplification of the critical temperature appears to be common in cuprates [5,6] pnictides, [7,8] diborides [9] although the large differences between these materials.

Shape resonances appear in systems made of multiple components, where the Fermi level is tuned near a Lifshitz critcal point in one of the bands. The complexity of the electronic and lattice phase of these materials arises because the system is in the verge of a catastrophe i.e. near a critical point for an arrested first order phase transition as shown in superoxigenated La2CuO4+y [10] showing scale free structural organization of percolating striped domains of oxygen interstitials favoring the high Tc phase.

[1] Antonio Bianconi,: "High Tc superconductors made by metal heterostructures at the atomic limit" European Patent No. 0733271 (published in European Patent. Bulletin 98/22, May 27 1998)) (priority date 7 Dec 1993);
and US Patent 6,265,019 (2001).

[2] Bianconi, A. On the possibility of new high Tc superconductors by producing metal heterostructures as in the cuprate perovskites. Solid State Communications 89, 933-936 (1994). URL http://dx.doi.org/10.1016/0038-1098(94)90354-9.

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[7] Caivano, R. et al. Feshbach resonance and mesoscopic phase separation near a quantum critical point in multiband feas-based superconductors. Superconductor Science and Technology 22, 014004+ (2009). URL http://dx.doi.org/10.1088/0953-2048/22/1/014004.

[8] Innocenti, D. *et al.* Shape resonance for the anisotropic superconducting gaps near a lifshitz transition: the effect of electron hopping between layers. *Superconductor Science and Technology* **24**, 015012+ (2011). URL http://dx.doi.org/10.1088/0953-2048/24/1/015012.

[9] Innocenti, D. *et al.* Resonant and crossover phenomena in a multiband superconductor: Tuning the chemical potential near a band edge. *Physical Review B* **82**, 184528+ (2010). URL http://dx.doi.org/10.1103/PhysRevB.82.184528.

[10] Fratini, M. *et al.* Scale-free structural organization of oxygen interstitials in La2CuO4+y. *Nature* **466**, 841-844 (2010). URL http://dx.doi.org/10.1038/nature09260.

Superconductivity and magnetism in iron pnictides.

Sergey Borisenko

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We study different iron-based superconducting materials at ultra low temperatures by means of angle-resolved photoemission spectroscopy. The measurements provide a direct access to the information on the low energy electronic structure, which includes the detailed knowledge of the Fermi surface, band renormalization, electronic self-energy and symmetry of the superconducting order parameter. The results suggest a direct correlation between the fermiology and fundamental physical properties throughout the phase diagram of iron superconductors.

Adiabatic and non-adiabatic phonon frequencies in a Wannier function approach:applications to CaC6, MgB2 and K-doped Picene.

M. Calandra[1], G. Profeta[2], M. Casula[1], and F. Mauri[1]

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We develop a Wannier-interpolation scheme to obtain well converged adiabatic and non-adiabatic phonon dispersions on extremely dense k-points grids from first principles. The method is particularly efficient in metallic systems displaying Kohn anomalies and long range force constants and, more generally, whenever a very good convergence with respect to Brillouin zone sampling and with respect to the electronic temperature is needed.
The developed Wannier-interpolation scheme is applied to the calculation of the phonon dispersion and electron-phonon coupling in MgB2, CaC6 and K-doped Picene (78 atoms per cell).
In MgB2 we show that a well converged calculation of the phonon frequencies is mandatory to obtain an accurate Eliashberg function. In CaC6 we show that a large number of Kohn anomalies occur on the phonon branches at all energy scale in the phonon spectrum. Furthermore we demonstrate that the high energy phonon modes (Carbon in-plane vibrations) display substantial non-adiabatic effects exteding over a large portion of the Brillouin zone. This non-adiabatic shift of the high energy modes should be visible with inelastic X-ray or Neutron scattering experiments.
Finally, in superconducting K-doped picene, we demostrate that intercalant and intermolecular phonon-modes contribute substantially (40%) to λ as also shown by the isotope exponents of potassium (0.19) and carbon (0.31). The relevance of these modes makes superconductivity in K-doped picene peculiar and different from that of fullerenes.

Adiabatic and nonadiabatic phonon dispersion in a Wannier function approach, M. Calandra, G. Profeta and F. Mauri, Phys. Rev. B **82**, 165111 (2010)
Intercalant and intermolecular phonon assisted superconductivity in K-doped picene, Michele Casula, Matteo Calandra, Gianni Profeta, Francesco Mauri, arXiv:1106.1446

Interband interactions and optical conductivity in iron-based superconductors.

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The new superconducting iron-based pnictides represent a new challenge in the field of condensed matter. Understanding the features of the scattering mechanisms related to the pairing is thus fundamental to control and exploit the superconducting properties. One of the main characteristics of these materials is certainly the role of the different Fermi pockets. First-principle calculations indeed identify four main bands at the Fermi level with twodimensional character: two hole-like pockets around the Γ point and two electron-like pockets around the M point, so that these systems present an interesting multiband phenomenology. Such multiband properties are also intrinsically related with a strong particle-hole asymmetry character in each band. In this contribution I will show how this scenario has important consequences on the phenomenology of the many-body interband interaction, thought to be the main responsible for the superconducting pairing. Focusing on the normal state, in particular, we will see how the optical conductivity is affected in a non-trivial way, with a redistribution of the intraband spectral weight between coherent and incoherent processes, resulting in a substantial conservation of the optical sum rule. The role of the interband transitions in the optical conductivity will be also examinated within the context of an extended Drude model analysis.

The electron-phonon coupling in strongly correlated solids studied by ultrafast techniques.

F. Carbone

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Ultrafast pulses of light allows to instantaneously drive the electronic as well as the crystal structure out of equilibrium. When this happens, the redistribution of energy in the solids occur in the fs to ps time-scale through electron-lattice interactions. The observation of the electronic structure through optical spectroscopy or photoemission yield the relaxation behavior of excited carriers, while the consequent structural rearrangements can be followed in diffraction experiments, either with electrons or X-rays. In this seminar, we review some results on strongly correlated solids and address the symmetry and strength of electron-phonon coupling. The relevance of these results for superconductivity will be also discussed.

Multiband Eliashberg Model for pnictides.

O. V. Dolgov[1], D.V. Efremov[1] , A.A. Golubov[2], A.V. Boris[1]

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[2]University of Twente, Enschede, The Netherlands

Existing experimental data demonstrate multiband character of ferropnictides. We study multiband Eliashberg model based on interband spin-fluctuation interaction. Within this model, superconducting gap functions have different signs on electronic and hole pockets, the so-called s_{+-} symmetry state. These states have a number of interesting features which manifest themselves in thermodynamics and transport properties. Using 4-band model, with 2 electronic and 2 hole pockets, we have calculated energy gaps and specific heat. These results are in a good agreement with experiments on K-doped pnictides. Further, we have studied impurity scattering outside Born approximation and have shown that nonexponential temperature dependencies of superfluid density and NMR relaxation rate can be realized. The origin of this behavior is explained by the fact that s_{+-} state, which is gapped in the clean limit, turns gapless when sufficient amount of impurity scattering is introduced.

Vibrational properties of MnO and NiO from DFT+U-based Density Functional Perturbation Theory.

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In this talk I will introduce a novel extension of Density Functional Perturbation Theory that allows self-consistent linear-response calculations from a DFT+U ground state. The scheme will be illustrated in the framework of ultrasoft pseudopotentials. Using this calculational method, the full phonon dispersion of strongly correlated materials, whose ground state can be captured with Hubbard-corrected functionals, can be accessed with very high accuracy and numerical efficiency. The new tool is applied to the study of MnO and NiO in their antiferromagnetic (AFII) ground state, showing that the Hubbard correction significantly improves the description of the vibrational properties of these systems, if compared to linear response calculations from LDSA/σGGA.

Strong impurity scattering in multiband superconductors.

A.A. Golubov[1], O.V. Dolgov[2], D.V. Efremov[2], M.M. Korshunov[3]

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We reexamine the problem of disorder in two-band superconductors, and show within the framework of the T -matrix approximation that the suppression of critical temperature Tc can be described by a single parameter depending on the intra- and interband impurity scattering rates. Tc is shown to be more robust against nonmagnetic impurities than would be predicted in the trivial extension of Abrikosov-Gor'kov theory. For some realizations of s± pairing in such systems, we find a disorder-induced transition from the s± state to a gapless and then to a fully gapped s++ state, which occurs at a critical value of the interband scattering rate. We discuss implications for experiments.

Directional point-contact Andreev-reflection spectroscopy of Fe-based superconductors: Gap symmetry and Fermi surface topology.

R.S. Gonnelli[1], M. Tortello[1], D. Daghero[1], G.A. Ummarino[1], V.A. Stepanov[2], Z. Bukowski[3], N.D. Zhigadlo[3], J. Karpinski[3], J. Jiang[4], P. Reuvekamp[5] and R.K. Kremer[5]

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The number and the symmetry of the order parameter(s) (OPs) in Fe-based superconductors, as well as the occurrence of anisotropic or nodal OP symmetries are important topics at the center of the present scientific debate. We show here that when accurate point-contact Andreev-reflection (PCAR) experiments in good-quality samples are carried out by different groups they do provide surprisingly consistent results. Moreover, the analysis of directional PCAR results in complex materials requires advanced theoretical tools. In this context we recently extended the theoretical model for Andreev reflection to the full 3D case accounting for Fermi surfaces of (almost) arbitrary shape. This combined theoretical/experimental approach allows us to conclude that, in the most studied La 1111, Sm 1111, Co-doped and K-doped Ba 122 compounds around optimal doping, the available high-quality PCAR results agree rather well on the presence of two isotropic gaps. On the other hand, our recent directional PCAR results on single crystals of the Ca 122 family clearly show the presence of at least one nodal (or strongly anisotropic) OP, possibly in agreement with recent theoretical predictions.

Electron-phonon coupling and superconductivity in bulk and thin films of lead: importance of relativistic corrections.

Rolf Heid[1], Klaus-Peter Bohnen[1], Irina Sklydneva[2], Evgeni Chulkov[2]

[1]Karlsruhe Institute of Technology, Institute for Solid-State Physics,
[2]Donostia International Physics Center, San Sebastian, Spain

Recent experimental evidence that superconductivity exists in Pb films even for thicknesses down to a few monolayers has renewed the interest in an accurate determination of the electron-phonon coupling (EPC) properties of bulk and thin metal films. Previous DFT-based linear-response calculations were restricted to a semi-relativistic framework, where spin-orbit coupling (SOC) is neglected. It was recently shown that for the prototypical strong-coupling superconductor Pb SOC significantly increases the EPC coupling constant λ by 44% [1], which solves the longstanding puzzle of too small λ values obtained consistently in previous first principles calculations. In this talk, I will first discuss the influence of SOC on other bulk properties like phonon-induced electronic self-energies and lifetimes. Then I will focus on EPC properties of thin Pb films, where in addition to SOC, the confinement of the electronic motion, i.e., the presence of quantum-well states, has an important impact on the overall EPC strength and superconducting properties.

[1] R. Heid, K.-P. Bohnen, I. Yu. Sklyadneva, E. V. Chulkov, Phys. Rev. B 81, 174527 (2010)

Unconventional superconductivity viewed by the functional renormalization group – recent applications.

Carsten Honerkamp

Institute for Theoretical Solid State Physics, RWTH Aachen University, JARA-FIT Fundamentals of Future Information Technologies

The functional renormalization group (fRG) has become a widely used theoretical method to explore low-temperature long-range ordering trends in low-dimensional interacting many-fermion systems. While initially, the main focus was on simple model systems like the two-dimensional Hubbard model, there are now several problems where more complex multi-band systems and materials-specific issues have been addressed using the fRG. In this talk, I will describe some fRG studies in the field of iron pnictide superconductors and the recent attempts to understand material trends for superconducting transition temperatures. I will also address some further-reaching issues around the construction of low-energy models for the study of many-body effects.

Magnetism, superconductivity and spin fluctuations in Fe-based superconductors.

Michelle Johannes[1], Igor Mazin[1], David Singh[2], David Parker[2]

[1]Naval Research
[2]Oak Ridge National Laboratory

Since the discovery of a high temperature superconducting transition in ferropnictides approximately two years ago, the highly magnetic character of these compounds and the close relationship between superconductivity and magnetism has been widely recognized and intensely studied. Initially, debate about the nature of the magnetism was split into two camps: localized moments (as in cuprates) and pure itineracy (a spin-peierls type transition). But closer investigation shows that magnetism in pnictides and in the related chalcogenides is between these two extremes, consisting of Hund's rule (or Stoner) derived moments on the Fe atoms. Using density functional theory (DFT) calculations, it is shown that the ordering mechanism is not Fermi surface driven and is also unlikely to be of superexchange origin. From a computational perspective, it can be explained how the magnetic and structural transitions are related and doping and pressure dependent quantities can be compared to experiment. Many quantities are well reproduced and explainable using DFT, though remaining questions need to be answered before magnetism, superconductivity and their relationship can be considered as understood. Spin fluctuations are widely understood to be the driving force behind the superconductivity with magnetic order as a competing, and therefore detrimental, phase. In this context, a spin fluctuation scheme, known as the nematic phase, could explain why the structural transition appears either in conjunction with or before the magnetic transition. Spin fluctuations are also likely related to the suppression of LRO order with pressure and doping.

Phase formation in quantum critical systems.

Andy Mackenzie

SUPA, School of Physics & Astronomy, University of St Andrews, North Haugh, St Andrews KY16 9SS, Scotland

In recent years it has become clear that novel phases often form in clean systems on the approach to quantum critical points. I will review some of these developments, discussing both superconducting and non-superconducting phases found in intermetallic alloys and in oxides.

Symmetry-allowed pairing states in overdoped 122 iron selenides.

I. I Mazin

Naval Research Laboratory

I will discuss the status quo of the most recent addition to the family of Fe-based superconductors, alkali-metal intercalated selenides with 122 crystal structure. I will first review the experimental situation, emphasizing the extent to which different experiments are so far inconsistent with each other, and what ramifications they may have to the filed. I will particularly concentrate of the ARPES experiments, the issue of the vacancy ordering and associated large-scale magnetism, and the phase diagram both with respect to doping and to the Fe vacancies concentration. In the second part I will discuss which superconducting symmetries, apart the trivial constant-sign s-wave, are compatible with the crystallographic constraints put forward by the KFe2Se2 general frame (not accounting for possible vacancy ordering).

Quantum size effects in nano-scale superconductors.

François Peeters

Departement Fysica, Universiteit Antwerpen, B-2020 Antwerpen, Belgiumemplate

Quantum confinement of electrons in metallic clean nanowires and nanofilms results in the formation of a series of subbands that move in energy with changing thickness. When the bottom of such a subband moves throught the Fermi surface, the density of states changes and a shape resonance appears leading to oscillations in the critical temperature, the critical magnetic field, the critical current and the size of the Cooper pairs as function of the wire/film width. Our theoretical formulation is based on a numerical solution of the Bogoliubov-de Gennes equations. A quantitative description is given of recent experimental data on the thickness dependence of Tc in Al and Sn nanowires and Pb nanofilms. At a shape resonance the density of the superconducting condensate in a superconducting nanowire is very inhomogeneous, leading to new Andreev-type of states. In the presence of a parallel magnetic field we predict that the superconductor-to-normal transition at zero temperature occurs as a cascade of subsequent jumps in the order parameter (this is opposed to the smooth second-order phase transition in the mesoscopic regime). Each jump is associated with the depairing of electrons in one of the single-electron subbands. Pronounced quantum-size oscillations of the critical magnetic field with giant resonant enhancements are predicted. The longitudinal distribution of electrons in a Cooper pair becomes strongly localized when the lower edge of one of the single-electron subbands is close to the Fermi surface. For nanowires made of conventional superconducting materials, the coherence length drops by two-three orders of magnitude and reaches values found in high-Tc superconductors. The underlying physics of this phenomenon suggests it will also be found in other superconducting/superfluid systems with a similar single-fermion spectrum, e.g. in ultrathin metallic nanofilms and atomic Fermi gases confined in a quantum-wire or quantum-well geometry. In the presence of a parallel magnetic field we predict that the superconductor-to-normal transition at zero temperature occurs as a cascade of subsequent jumps in the order parameter (this is opposed to the smooth second-order phase transition in the mesoscopic regime). Each jump is associated with the depairing of electrons in one of the single-electron subbands. Pronounced quantum-size oscillations of the critical magnetic field with giant resonant enhancements are predicted.

* Work done in collaboration with A. Shanenko and M. Croitoru

Review paper: F. M. Peeters, A. A. Shanenko, and M. D. Croitoru: Nanoscale superconductivity, in "Handbook of Nanophysics: Principles and Methods", Editor. Klaus D. Sattler (Taylor & Francis Publisher (CRC Press), 2010), p. 9-(1-31).

How to make graphene superconducting.

G. Profeta [1], M. Calandra[2] and F. Mauri[2]

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[2]IMPMC, Université Paris 6, CNRS, 4 Pl. Jussieu, 75015 Paris, Franceemplate

Graphene is the physical realization of many fundamental concepts and phenomena in solid state-physics, but in the long list of graphene remarkable properties, a fundamental block is missing: superconductivity. Making graphene superconducting is relevant as the easy manipulation of this material by nanolytographic techniques paves the way to nanosquids, one-electron superconductor-quantum dot devices, superconducting transistors at the nano-scale and cryogenic solid-state coolers.

Here we explore the doping of graphene by adatoms coverage. We show that the occurrence of superconductivity depends on the adatom in analogy with graphite intercalated compounds (GICs). However, most surprisingly, and contrary to the GIC case, Li covered graphene is superconducting at much higher temperature with respect to Ca covered graphene.

State of the art and new developments in superconducting density functional theory.

Antonio Sanna

Max Planck Institute for Microstructure Physics: 06120 Halle(Saale) Germany

I will review the theoretical framework of superconducting density functional theory (SCDFT), a fully parameter-free approach to superconductivity. The advantages and disadvantages of this method will be presented, as well as more recent extensions and perspectives.

First I will present the connection of the theory to Eliashberg's method, and discuss some exact limits. Then I will report on how this connection can be used to improve the existing phononic functionals.

The purely electronic part of the coupling in SCDFT will also be analyzed and properties and limits of the static random phase approximation will be discussed. Finally I will report on recent extensions which include dynamical effects in the screened interaction.

Superconductors Near Magnetism.

David J. Singh

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Understanding the interplay of magnetism and superconductivity in specific materials is a longstanding challenge. Nonetheless, the ability to do first principles calculations of relevant physical properties of specific materials has contributed much understanding of the likely mechanisms in different cases, as well as opening a number of questions. Here specific materials -- borocarbides, MgCNi3, ruthenates and Fe-based materials -- are discussed from this point of view. Open questions are emphasized.

*Supported by the Department of Energy, Office of Science, Materials Sciences and Engineering Division

Spectral and magnetic properties of the iron-based superconductors: The role of electronic correlations.

A.Toschi[1], P. Hansmann[1], R. Arita[2], S. Sakai[1], G. Sangiovanni[1], K. Held[1]

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Electronic correlation plays a subtle role in Fe-based superconductors. In fact, due to the presence of several moderately correlated bands close to the Fermi level, one observes the formation of localized magnetic moments driven by the Hund's exchange interactions, which takes place, however, in a mainly metallic background ("Hund's metal"[1]). This physical scenario provides the key to understand[2,3] the discrepancies observed between experimental estimates of the magnetic moments in the magnetically ordered phase and those obtained via standard LSDA calculations. The magnitude of the discrepancy observed in different compounds would be hence related to the efficacy of the metallic screening, which is decreasing when going from the 1111 (e.g., LaFeAsO) to the 122 class, and eventually to the 11 materials (like FeTe).

Also important to be considered for the interpretation of the ARPES experiments and of the symmetry of the superconducting pairing within the Hunds' exchange scenario is the interplay between the electronic correlations and the details of the band-structure of the specific compound considered.

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[3] P. Hansmann, R. Arita, G. Sangiovanni, A. Toschi & K. Held, in preparation.

Electron-Phonon Coupling From Finite-Displacement Approach: A Case Study for Metal Doped Picene and Fe-based Superconductors.

Taner Yildirim*

NIST Center for Neutron Research, Gaithersburg, MD, USA and
Department of Materials Science and Engineering, University of Pennsylvania, PA

The standard linear response theory has been successfully used to calculate el-ph coupling in systems with few atoms. However when the system size is large and/or magnetism and phonons are strongly coupled as found in Fe-based superconductors, the linear response approach may not be feasible. Hence, we have developed a finite-displacement method where both the phonon energies and el-ph coupling can be easily calculated for large systems with and without magnetism. In this talk, after a brief overview of finite displacement approach, we will apply this method to study el-ph coupling in two recent classes of superconductors; namely alkali-doped solid Picene (T_c~ 18 K) and magnetic Fe-based superconductors. For the case of K_3Picene, in agreement with our inelastic neutron data, we found very strong electron-phonon coupling for the intra-molecular phonons. This coupled with almost flat electronic bands yields very high Tc for Picene while no superconductivity is predicted for Pentacene. We discuss the effect of charge transfer as well as pressure on Tc for solid Picene and make predictions for new superconductors based on other small hydrocarbon molecular systems. In the last part of the talk, we will discuss spin-resolved electron-phonon coupling in various iron-based superconductors.

* The work was done in close collaboration with Xuhui Luo and S. Ogut, Physics Department, University of Chicago at Illinois.

Posters

Like in this booklet, the posters are displayed in alphabetical order according to the presenting author.

Dirac cones states at La(Fe,Ru)AsO.

F.Bernardini [1], I.Pallecchi [2], M.Tropeano [2,5], C.Ferdeghini [2], A.Martinelli [2], M.Vignolo [2], A.Palenzona [2,3], S. Massidda[1], M.Putti [2,4]

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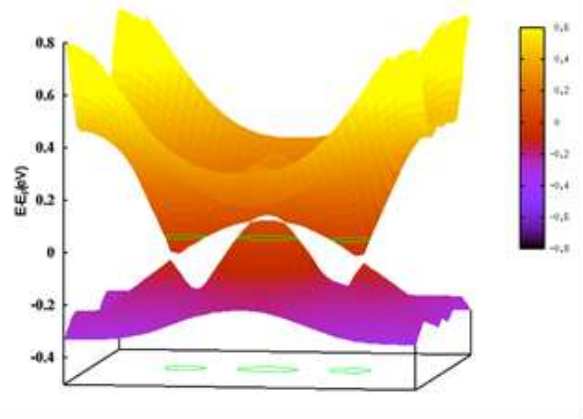
Dirac fermion states are one of the most intriguing issue in condensed matter physics. These massless states are found in graphene, topological insulators, and organic conductors. Abrikosov showed that Dirac cone (DC) states can be identified by the low temperature behavior of the magneto-resistance [1]. In additon to the usual quadratic dependence of (□(H)-□(H=0))/□(H=0) on magnetic field, a linear dependence appears in the presence of DC states. Such a behavior was discovered in experiments of magneto-resistance in BaFeAs [2] and Pr(Ru,Fe)AsO [3] supporting the existence of Dirac cone (DC) states in other iron-pnictides superconductors too. Theoretical investigation shows that DC are formed by the folding of the d-band due to antiferromagnetic order and survive the gap opening effect of spin-density wave (SDW) [4]. Spurred by this finding we investigate the issue of DC states in LaFe1-xRuxAsO ($0 \leq x \leq 0.6$). We find out that in the whole series: (i) the transport is dominated by electron bands only; (ii) the magnetoresistance exhibits distinctive features related to the presence of Dirac cones; (iii) ab initio calculations confirm the presence of anisotropic Dirac cones in the band structure; (iv) the low temperature mobility is exceptionally high and reaches 18.6 m2/(Vs) in the Ru-free sample at T=2K, in the extreme limit of a single Landau level occupied in the Dirac cones; (v) the mobility drops abruptly above 10K-15K; (vi) the disorder has a very weak effect on the band mobilities and on the transport properties. These findings may be of crucial importance in the investigation of the pairing mechanism in the F-doped superconducting La(Fe,Ru)As(O,F) compounds related to this series of parent compounds.



Ab initio approach to magnon-electron scattering.

Paweł Buczek[1], Frank Essenberger[1], Paolo E. Trevisanutto[1], Christophe Bersier[1], Arthur Ernst[1], Leonid M. Sandratskii[1], Evgueni V. Chulkov[2], E.K.U. Gross[1]

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The electronic properties of magnets and exchange-enhanced paramagnets are strongly influenced by the spin-flip fluctuations. In particular, they may play a role in the mechanism of superconductivity in the pnictide and cuprate superconductors [Mazin & Johannes, Nat. Phys. 5, 141 (2009)].

We combine time dependent linear response density functional theory of magnetization fluctuation [Buczek et al., Phys. Rev. Lett. 105, 097205 (2010)] with the methods of many body perturbation theory [Vignale & Singwi, Phys. Rev. B 32, 2156 (1985); Zhukov et al., Phys. Rev. Lett. 93, 096401 (2004)] to obtain an effective electron-electron interaction involving emission and absorption of magnons.

The theory is applied to recent inelastic tunneling spectroscopy experiments [Balashov et al., Phys. Rev. Lett. 97, 187201 (2006)] and to the magnon mediated Cooper pair formation in PdH, LaFeAsO and FeSe.

Intercalant and intermolecular phonon assisted superconductivity in K-doped picene.

Michele Casula[1], Matteo Calandra[1], Gianni Profeta[2], Francesco Mauri[1]

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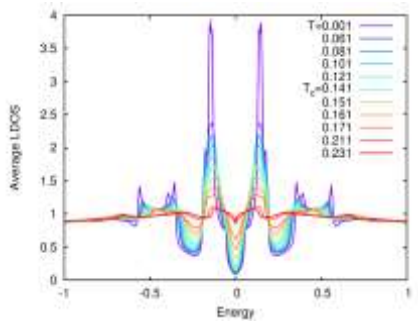
K_3-picene is a superconducting molecular crystal with critical temperature T_c = 7 K or 18 K, depending on preparation conditions. Using density functional theory we show that electron-phonon interaction accounts for T_c ~ 3-8 K. The average electron-phonon coupling, calculated by including the phonon energy scale in the electron-phonon scattering, is λ=0.73 and ω_{log}=18.0 meV. Intercalant and intermolecular phonon-modes contribute substantially (40%) to λ as also shown by the isotope exponents of potassium (0.19) and carbon (0.31). The relevance of these modes makes superconductivity in K-doped picene peculiar and different from that of fullerenes.

Proximity effect in the presence of phase fluctuations.

Lucian Covaci and Francois Peeters

Universiteit Antwerpen, Belgium

Phase fluctuations in high-Tc superconductors are believed to play an important role in the underdoped regime. Various experimental measurements (Nernst effect, STM, resistivity, etc.) suggest that a superconducting state which has a finite order parameter but acquires a disordered phase is responsible for the peculiar properties of the pseudogap regime. Recently, STM measurements [1] on structures made of superconducting LSCO put in contact with a metallic layer (either overdoped LSCO or Au) revealed that the STM gap located at the Fermi level survives above the superconducting critical temperature when the LSCO layer is in the pseudogap phase. The location of the gap remains pinned to the Fermi level even if the nature of the metallic layer is changed (overdoped LSCO or Au). In a previous study [2] we showed that a gap induced by spin density wave order will not follow the Fermi level when the band structure of the metallic layer is modified. One needs an order with Q=0 in order to explain the experimental findings, such an order is the phase fluctuating superconductor. We consider a model in which the mean-field transition temperature is higher than the phase ordering temperature. Regions with size on the order of the coherence length are next considered as spins in a 2D-XY model which will have a lower critical temperature. Using a Monte-Carlo procedure for the 2D-XY model we extract for each temperature a set of phase configurations with which we compute the average LDOS at the surface of the metallic layer. We show that at the phase ordering temperature there is little change in the LDOS gap, similar to experimental findings. Above the phase ordering temperature vortex-anti vortex pairs will be unbound and rapid changes of the phase will induce zero energy bound states in the metallic region which will then, on average, fill the LDOS gap. Due to the requirement of large system size needed in order to describe the proximity effect in this system we use the Chebyshev-BdG method [3] previously developed in our group. The Chebyshev-BdG methods is expanded to computations on Graphics Processing Units (GPU) to give impressive speed-up times (on the order of x1000 on a server with three GTX 580 GPUs).



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Multiple gaps and strong electron-boson interaction in Fe-based superconductors: a point-contact Andreev-reflection study.

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We show that the results of point-contact Andreev-reflection (PCAR) measurements carried out by us and other groups in 1111 and 122 Fe-based compounds (such as LaFeAs(O,F), SmFeAs(O,F), $(Ba,K)Fe_2As_2$ and $Ba(Fe,Co)_2As_2$) consistently indicate – if analyzed in a homogeneous way – the existence of (at least) two nodeless and presumably isotropic gaps, whose values can be reproduced within a $s\pm$ Eliashberg model. Many of the best PCAR spectra show additional structures (at energies higher than the gaps) that are not accounted for by the BTK models used to fit the experimental curves. We show that these features are due to the strong electron-boson interaction and can be reproduced by inserting in the BTK model the order parameters $\Delta_i(E)$ obtained within the $s\pm$ Eliashberg model by using an electron-boson spectral function $\alpha^2F(\omega)$ peaked at a suitable energy Ω_0. In $Ba(Fe,Co)_2As_2$, Ω_0 turns out to coincide with the spin-resonance energy measured by inelastic neutron scattering, which strongly supports a spin-fluctuation mediated pairing. In SmFeAs(O,F) we obtain Ω_0=20 meV, that is $\Omega_0 \cong 4.65 k_B T_c$, in agreement with what inferred from neutron scattering results on other Fe-based superconductors

Janus-faced influence of Hund's rule coupling in correlated materials.

Luca de' Medici

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We show that in multi-band metals the correlations are strongly affected by the Hund's rule coupling, which depending on the filling promotes metallic, insulating or bad-metallic behavior. The quasiparticle coherence and the proximity to a Mott insulator are influenced distinctly and, away from single- and half-filling, in opposite ways. A strongly correlated bad-metal far from a Mott phase is found there.

We propose a concise classification of 3d and 4d transition-metal oxides within which the ubiquitous occurrence of strong correlations in Ru- and Cr-based oxides, as well as the recently measured high Neel temperatures in Tc-based perovskites are naturally explained.

ArXiv: 1106.0815

Superconducting Density Functional Theory Bootstrap Method.

J. K. Dewhurst, S. Sharma, A. Sanna and E. K. U. Gross

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We present a method for solving the superconducting density functional theory problem formally exactly. In the first step, initial normal and anomalous densities, $\rho(\mathbf{r})$ and $\chi(\mathbf{r},\mathbf{r}')$, are chosen. Then the non-interacting Kohn-Sham-Bogoliubov-de Gennes (KSBdG) equations are inverted to determine the conjugate Hartree-exchange-correlation potentials $v_{Hxc}(\mathbf{r})$ and $\Delta_{xc}(\mathbf{r},\mathbf{r}')$. These potentials are then added to and subtracted from the full Hamiltonian, and finite temperature many-body perturbation theory is employed to some order in the interaction $\hat{H}_I \equiv \hat{V}_{e-e} + \hat{V}_{e-ph} - \hat{V}_{Hxc} - \hat{\Delta}_{xc}$, where $\hat{V}_{e-e}$ is the electron-electron interaction and $\hat{V}_{e-ph}$ is the electron phonon interaction, to find the normal and anomalous Green's functions $\mathscr{G}(\mathbf{r},\mathbf{r}',\omega)$ and $\mathscr{F}(\mathbf{r},\mathbf{r}',\omega)$. New densities are constructed from these using $\rho(\mathbf{r}) = \beta^{-1}\sum_n e^{i\omega_n 0^+}\mathscr{G}(\mathbf{r},\mathbf{r},\omega_n)$ and $\chi(\mathbf{r},\mathbf{r}') = \beta^{-1}\sum_n e^{i\omega_n 0^+}\mathscr{F}(\mathbf{r},\mathbf{r}',\omega_n)$ and the proceedure is repeated until self-consistency is achieved. This method places the burden of finding the exchange-correlation potentials on the numerical inversion of the KSBdG equations, rather than on analytic functional derivatives of the exchange-correlation energy. The effect of self-consistency is in the proceedure 'bootstrapping' itself into the broken symmetry phase, and we make a comparison of this approach to renormalization group methods.

Strong Impurity Scattering in two-band Superconductors.

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We have reexamined the problem of nonmagnetic and magnetic impurities in two-band superconductors. Tc is shown to be more robust against nonmagnetic impurities than would be predicted in the trivial extension of Abrikosov-Gorkov theory. For some realizations of s+- pairing in such systems, we find that a disorder-induced transition between the s+- states to a gapless and then to a fully gapped s+- state, which occurs at a critical value of the interband scattering rate. We discuss how this transition can manifest itself in the behavior of the electronic density of states and some thermodynamical properties as the magnetic field penetration depth.

Spin Excitations in Density Functional Theory for Superconductors.

Frank Essenberger[1], P. Buczek[1], A. Ernst[1], J. K. Dewhurst[1], A. Sanna[1] and E.K.U. Gross[1]

[1]Max Planck Institute of Microstructure Physics in Halle, Germany

In the density functional theory (DFT) approach for superconducting (SC) materials the anomalous density , χ, is introduced as an extra basic variable. All ground state expectation values then become functionals of the electronic density ρ as well as χ: In the SC Kohn–Sham system the conjugate potential Δ_{xc} defined by $\delta E_{xc}/ \delta\chi$ couples to this density χ [3].
Currently the perturbation expansion for Δ_{xc} includes terms up to first order in the phonon propagator and the static screened Coulomb interaction within the random phase approximation ω^{RPA} [1]. However for unconventional superconductors this approach fails. One possible reason for this failure is related to the fact that in these materials the Cooper-pairing is mediated by spin excitations [2]. We present a way to include these spin fluctuations and excitations in the framework of SC-DFT. Following the approach of Vignale et al. [4] a replacement for ω^{RPA} is derived. The new effective electron–electron interaction is spin dependent. It includes the contribution of charge fluctuations as well as longitudinal and transverse spin fluctuations.

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Analysis of bosonic structures in tunnel and Andreev-Reflection spectroscopy by solutions of Eliashberg equations.

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The tunnelling and the Andreev-reflection conductance spectra show structures related to the electron-boson interaction from which the boson characteristic energy can be obtained. By solving the Eliashberg equations we analyzed the position of these structures, which appear in the density of states in the case of single and multiband superconductors with particular attention to the effect of the shape of the spectral function. We show that the first peak in the sign-changed first derivative of the conductance is closely related to the spectral function peak, regardless of the spectral function behaviour at low energies and of the single or multiband nature of the superconductivity of the system. We also analyzed Andreev-reflection measurements in Fe-based superconductors where we were able to extract the boson representative energy and its temperature dependence, as well as to reproduce the experimental curves by solution of the Eliashberg equat

Real-space structure of the superconducting order parameter.

A. Linscheid[1], A. Sanna[1], A. Floris[2], E.K.U. Gross[1]

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[2]King's College -London, United Kingdom

Superconductors are usually characterized by global features as the critical temperature, the specific heat or the gap on the Fermi surface (FS). How these properties are related to microscopic features, such as chemical bonds, is not well understood. In this study we have calculated the superconducting (SC) order parameter (OP) and the gap function in real space for the materials MgB2, CaC6 and a mono-layer of SC graphane and investigated their microscopic structure. The calculations are performed using SC density functional theory, a method with no free parameters fitted to experimental data representing the ideal framework to investigate the microscopic structure of the OP from first principles. We find that the OP's magnitude varies drastically in the unit cell thus yielding an even higher difference in the pair distribution function of the SC phase. The dependence of the OP on the relative spacing between the SC electrons is found to be oscillating which we can explain by the shape of the FS in these materials.

Symmetry analysis of Noncentrosymmetric Superconductors LiPdxPt3−xB, MoAl3C2 and α-BiPd.

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[2]ISIS facility, STFC Rutherford Appleton Laboratory
[3]SEPnet and Hubbard Theory Consortium, University of Kent

The recent interest in noncentrosymmetric (NCS) superconductivity has been triggered by the discovery of superconductivity in the NCS heavy-fermion compound CePt3Si. In this and other NCS superconducting materials the lack of inversion may allow for an admixture of singlet and triplet pairing *via* spin-orbit coupling (SOC). The available pairing symmetries for a given crystal point group can be classified in all generality
using group theory. Here we present such analyses for the NCS point groups *O* and *C*2. The first of these groups corresponds to the NCS superconductors LiPd*x*Pt3−*x*B, where the strength of SOC, and therefore the degree of singlet-triplet admixture, can be continuously tuned by doping; and to the more recently discovered MoAl3C2, whose pairing symmetry is at present unclear. The latter point group describes the
even more recently-discovered NCS superconductor *α*-BiPd. This is a particularly interesting point group on account of its very low symmetry. The role of spin-orbit coupling and the possibility of time-reversal symmetry breaking in these systems will be discussed.

Superconductivity by Ginzburg-Landau simulations.

M.V. Milošević*

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In this presentation, I will review the applicability and accomplishments of the mean-field Ginzburg-Landau theory in the studies of vortex matter and critical parameters of bulk, mesoscopic and nanoscale superconductors, also single- and multi-band materials. The numerical experimentation provided by the Ginzburg-Landau model is arguably the most useful theoretical tool in superconductivity for a quick and detailed insight into the essential properties of the superconducting condensate on a mean-field level. As such, this technique is fully complementary to the experimental efforts in the field, as it allows for sample nanostructuring (by e.g. perforations or magnetic hybridization) and (zero) field-cooling procedure in the very same manner as in the experiment, but provides information invisible for individual experimental techniques. I will demonstrate exactly how and to which extent the Ginzburg-Landau numerics compares to the transport, magnetic and scanning-tunneling measurements, illustrated by the recent examples and publications on vortex statics and dynamics.

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Structural and magnetic properties of FeTe under hydrostatic pressure within density functional theory.

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We report on first principle calculations of the structural and magnetic properties of FeTe under hydrostatic pressure, within density functional theory (DFT). We carefully examined several possible different crystal structures over a pressure range up to ~30GPa: simple tetragonal (PbO type), simple monoclinic, orthorombic (MnP type), hexagonal (NiAs and wurzite type) and cubic (CsCl and NaCl type). For each phase we examined the most likely magnetic orderings. Our calculation confirms the low temperature zero pressure ground state to be an antiferromagnetically ordered double stripe, in agreement with the experimental and previous theoretical calculations. Increasing pressure from zero is found to suppress magnetism (at around 17GPa) and simultaneously to drive the system through different magnetic ordering (notably also some ferromagnetic phases).

Competition between Electron-Phonon coupling and Spin Fluctuations in superconducting hole-doped CuBiSO.

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CuBiSO is a band insulator that becomes metallic upon hole doping. Superconductivity was recently reported in doped $Cu_{1-x}BiSO$ and attributed to spin fluctuations as the pairing mechanism. Based on first principles calculations of the electron-phonon coupling, we argue that the latter is very strong in this material, and probably drives superconductivity. The critical temperature is however strongly depressed by the proximity to magnetism. Thus, $Cu_{1-x}BiSO$ is a quite unique compound where both a conventional phonon-driven and an unconventional triplet superconductivity are possible, and compete with each other. We argue that, in this material, it should be possible to switch from conventional to unconventional superconductivity by varying such parameters as doping or pressure.

Multi-band Gutzwiller theory for iron pnictides.

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For the iron pnictide LaOFeAs we investigate multi-band Hubbard models which are assumed to capture the relevant physics [1,2]. In our calculations, we employ the Gutzwiller variational theory which is a genuine many particle approach [3]. We will present results both on the paramagnetic and antiferromagnetic phases of our model systems. These results show that a five band-model is not adequate to capture the relevant physics in LaOFeAs [4]. However, our results for the eight band-model which includes the arsenic 4p bands reproduce the experimental data, especially the magnetic moment, for a broad parameter regime.

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Self-consistent exchange-correlation kernel for time-dependent density functional theory.

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A new approximation for the exchange-correlation kernel within time - dependent density functional theory is proposed. This kernel is expressed as an algorithm in which the exact Dyson equation for the response as well as a further approximate condition are solved together self-consistently leading to a simple parameter-free kernel. We apply this to the calculation of optical spectra for various small bandgap (Ge, Si, GaAs, AlN, TiO_2, SiC), large bandgap (C, LiF, Ar, Ne) and magnetic (NiO) insulators. The calculated spectra are in very good agreement with experiment for this diverse set of materials, highlighting the universal applicability of the new kernel.

Linear-temperature dependence of static magnetic susceptibility in iron pnictides from dynamical mean-field theory.

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We present the LDA+DMFT (method combining Local Density Approximation with Dynamical Mean-Field Theory) results for magnetic properties of the parent superconductors LaFeAsO and $BaFe_2As_2$ in the paramagnetic phase. Calculated uniform magnetic susceptibility shows linear dependence at intermediate temperatures in agreement with experimental data. For high temperatures susceptibility first saturates and then decreases with temperature. Our results demonstrate that linear-temperature dependence of static magnetic susceptibility in pnictide superconductors can be reproduced without invoking antiferromagnetic fluctuations.

Solid picene: a possible exotic electron-phonon superconductor.

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We study superconductivity in doped solid picene (C22H14) with linear response calculations of the phonon spectrum and electron-phonon interaction. We show that the coupling of the high-energy C bond-stretching phonons to the *pi* molecular orbitals for a doping of ~3 electrons per picene molecule is sufficiently strong to reproduce the experimental T_c of 18 K within Migdal Eliashberg theory. However, the energy of strongly coupled phonons (~200 meV), bandwidth of the conduction bands (*W* ~0.3–1 eV), the ep coupling strength (*Vep*~110-150 eV) and Coulomb repulsion (*U*~1.2 eV)
all have similar magnitudes. Therefore, picene may belong to the same class of strongly correlated electron-phonon superconductors as fullerides, and we propose experimental tests for this hypothesis.

Is contact potential the hallmark of interaction in dilute Fermi gases?

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We develop a theoretical method to describe contact interaction in mean-field theories of many-fermion systems, using the low-energy *T*-matrix of the pair potential to rigorously define the effective radius of the interaction. One of the main consequences of our approach is the possibility to investigate finite-density effects, which are outside the range of validity of approximations based on δ-like potentials. We apply our method to the calculation of density dependent properties of an ultracold gas of ^{6}Li atoms at unitarity, whose two-body interaction potential is calculated using *ab initio* quantum chemistry methods. We find that density effects will be significant in ultracold gases with densities one order of magnitude higher than those attained in current experiments.

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