

**0.1 Report on Workshop Superconductors by the  
Mediterranean Sea: Classic and Novel Materials,  
Electronic States and Critical Properties**



**Hotel Porte Conto, Alghero, Sardinia, Italy**

**7-11 September 2009**

**Psi-k, ESF (INTELBIOMAT), CCP9, SLACS  
(CNR-INFN, Cagliari)**

**James Annett and Sandro Massidda**

**<http://www.phy.bris.ac.uk/groups/theory/psi-k-superconductivity.html>**

The theme of the workshop is ab initio theory of superconductivity, particularly based upon the recent developments of functionals for superconducting DFT. We also address exotic superconducting materials, and nanoscale devices in which normal state DFT calculations are used as the input for constructing models of the superconducting state and transport properties.

The main topics were, Electron-phonon coupling in low temperatures superconductors, Methodological improvements for calculating SC properties, Superconductivity at the nanoscale, Normal and superconducting state of HTS cuprates, Role of electron-phonon coupling in SC compounds and Unconventional superconductivity. In addition the workshop brought together theorists and experimentalists working on superconducting materials. The main experimental themes were electronic quasiparticle states, as measured in ARPES, transport and Fermi surface geometries, as measured in de Hass van Alphen and related experiments, and probes of the superconducting gap in muSR, tunnelling and Andreev point contact experiments.

The first day of the conference focussed on high temperature superconductors and the recently discovered pnictide family of superconducting materials. Lilia Boeri gave an excellent presentation on the work of the Stuttgart group. She started by reviewing the phase diagrams and structures of the various pnictide materials. She then presented the results of DFT calculations, including calculation of electron-phonon coupling constants, magnetic moments and the exchange gap as a function of the antiferromagnetic moment. The work demonstrated that electron-phonon coupling cannot account for the high transition temperatures observed in the Fe based pnictide materials. Furthermore the Stoner exchange parameter estimated from LDA was found to be too large to account for the experimental moment. Dr Patrick Rourke presented the first experimental talk, reviewing the angle dependent magnetoresistance measurements of the Bristol group on high  $T_c$  superconductors. He showed that in the Tl2201 materials there is clear evidence for a large cylindrical Fermi surface, in agreement with ARPES and band structure calculations. A detailed analysis of the data suggested a strongly  $k$  dependent electron scattering rate, which has both Fermi liquid-like  $T^2$  temperature dependent components as well as  $k$  dependent components having a non Fermi-liquid linear in  $T$  temperature dependence. Experimental results on the LSCO family of superconductors suggested a similar  $k$  and temperature dependence, however it was also necessary to include a term to account for resistivity saturation. The temperature-doping phase diagram shows broad regions of Fermi liquid  $T^2$  and non Fermi-liquid  $T$  temperature dependencies, but no evidence for a quantum critical point as a function of doping underneath the superconducting ‘dome’ region. The magnetism in the pnictide materials was also the subject of the talk given jointly by Christophe Bersier, John Kay Dewhurst and Sangeeta Sharma. The key point was that existing density functionals, such as GGA, do a bad job of structural optimization in these materials, and that the precise structural parameters are very closely linked to the magnetic states. Using a full potential LAPW method, they studied the various non-collinear magnetic states, such

as checkerboard, stripe, and 2K antiferromagnetism, and their dependence on doping and Fermi level in the materials.

In the afternoon session Dr Samuele Sanna discussed both pnictides and cuprate materials as studied in  $\mu$ SR experiments. In the cuprates the experiments were able to establish two types of magnetic behaviour once the antiferromagnetic order is destroyed by doping, these are a ‘frozen spin fluctuation’ regime and a spin-glass regime. A small coexistence region of these two states was also observed. In the pnictide materials the  $\mu$ SR experiments indicate that superconductivity and antiferromagnetism coexists only for a very small part of the phase diagram, and that the nature of the coexistence could be in nanoscale magnetic clusters consistent with scanning tunnelling microscopy experiments. Sergey Borisenko provided a very impressive overview of ARPES experiments in superconductors and related compounds, including investigations of the charge density wave material TaSe<sub>2</sub>. For BSCO he showed that the kink in the band dispersion near to the Fermi level can be used to deduce both the bosonic mode energy and electron-bosonic mode coupling parameter  $\lambda$ . These appeared consistent with interpreting the mode as spin fluctuation derived, but not as a phonon. Other experiments were shown for the ruthenate Sr<sub>2</sub>RuO<sub>4</sub>, and the CDW materials TaSe<sub>2</sub> and NbSe<sub>2</sub>. For the latter the measured Fermi surface appears to be inconsistent with the predictions from LDA. He also presented very exciting prospects for the science that will be achieved with the new 1-cubed instrument, which should obtain spectra at 1K with 1meV resolution. Finally Prof Wysokinski described the spin-triplet superconductor Sr<sub>2</sub>RuO<sub>4</sub> and the proposed gap function and three band model for chiral p-wave superconductivity in this material. He showed that orbital dependent superconductivity leads to distinct features the the NMR spectra for Ru and O nuclei, which can be used to help determine the structure of the gap function. A spin-flop type rotation of the superconducting d-vector was also found for a c-axis oriented field.

On the second day A. Floris began with a very clear summary of the achievements of the ab initio superconducting DFT theory, especially its predictions for  $T_c$  and gap values in classic superconductors and in MgB<sub>2</sub>. As a novel example of the theory Dr Floris presented results for Cmca phase of high pressure molecular hydrogen, which led to the prediction of  $T_c = 242$ K at a pressure of 450GPa. In the next talk Prof M. Calandra described first principles calculations on the CDW compound 2H-NbSe<sub>2</sub>. He predicted that both bilayer and single-layer NbSe<sub>2</sub> undergo a CDW instability. However in the bilayer, as in the bulk, the instability leads to a metallic state, while in the single-layer material it leads to a semimetallic ground state, in agreement with recent experimental data. Claudia Ambrosch-Draxl presented the results of electron-phonon coupling calculations obtained in the LAPW

method. The results compare well with the classic work of Engelsberg and Schrieffer, 1963, and shows a complex dispersion of models and subbands as the electron band dispersion crosses the phonon frequency. This was illustrated explicitly for calculations of H vibrational modes on W(001). For the high  $T_c$  cuprates the lattice instabilities and structural phase transitions in  $\text{La}-2-x\text{Sr}_x\text{CuO}_4$  led to imaginary phonon frequencies in the ideal tetragonal structure. An analysis of the Hubbard  $U$  led to the suggestion that GGA+ $U$  calculations were able to get an estimate of  $U$  as a function of doping,  $x$ , which in turn, led to a reasonable magnetic moment per Cu of  $\sim 0.6\mu_B$  per copper.

In the afternoon of the second day Rolf Heid reported his extensive first principles study of the electron-phonon coupling in  $\text{YBa}_2\text{Cu}_3\text{O}_7$  in the framework of the local density approximation (LDA). From this analysis he reported that the phonon-induced self-energy is about a factor 5 too small compared to the one estimated from experiments on the ‘kink’ in the ARPES quasiparticle dispersion curves. The phonon-induced pairing potential was calculated for both s and d-wave pairing channels and was found to be especially weak for pairing in the d-wave channel, strongly implying that this is not the source of the high  $T_c$  superconductivity. Marina Putti reported results for experimental measurements of the upper critical field,  $H_{c2}$  in pnictide superconductors. The anisotropy parameter  $H_{c2}^{ab}/H_{c2}^c$  was determined in several families of pnictide superconductors, including 1111, 122, and 11 materials. based on Fe layers have been discovered. It was found that the 1111 family shows larger  $T_c$  and anisotropic upper critical field, while the 122 family is less anisotropic. Finally the 11 family has the lowest  $T_c$ , it is nearly isotropic, but with a huge  $H_{c2}$  slope.

On the final day Prof Gonnelli described Andreev point contact experiments to elucidate the multiple gap structures in the Fe-As superconductors. The experiments seem to point clearly to two gaps, each of which is nodeless. Interestingly the larger gap can be as large at  $2\Delta/k_B T_c \sim 9$ , while the smaller one has  $2\Delta/k_B T_c \sim 5$ . Fitting the detailed temperature dependence to a three band Eliashberg theory can be obtained, but required very large values of the coupling constants  $\lambda$ . Prof Zwicknagl described the complex phase diagrams of layered organic superconductors exhibit. In particular she argued that the phase which separates the homogeneous superconducting state from the normal state is a realization of an inhomogeneous Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, based upon the upturn of the  $B_{c2}$  phase transition, which exceeds the paramagnetic limiting field, at low temperatures.

The session on nanoscale and non-equilibrium superconductivity was limited to just a single talk, by E. Perfetto. He described a new approach to

calculations of non-equilibrium transport in a model S-N-S junction, designed to model a nanoscale device with superconducting quantum point contacts. The Andreev states and their contribution to the total current was determined, as was the Josephson effect current as a function of external phase difference between the superconducting leads. A novel time evolution of the time-dependent Bogoliubov-deGennes equations was used to obtain the non-equilibrium Green's function, from which one could see both transient and steady state regimes, the latter agreeing with the Landauer formalism results. The transient effects clearly showed the effects of multiple Andreev reflections.

The final talk of the workshop was given by another experimentalist, Prof Andy Mackenzie. He reviewed experiments on Fermi surface and superconductivity in  $\text{Sr}_2\text{RuO}_4$ , and in particular on the effort to use the experimental de Haas - van Alphen effect is being used to measure the influence of spin-orbit coupling on its Fermi surface. He also described the metamagnetic phase diagram and search for a quantum critical point in  $\text{Sr}_3\text{Ru}_2\text{O}_7$ . In this material recent STM results in collaboration with J.C. Davis have produced the first real-space imaging of a Wannier function in a very strongly renormalized 'heavy' d-electron Fermi liquid as well as a field-induced transition to an electronic liquid-crystalline nematic like phase.

Altogether the workshop had an excellent mix of experimental and theoretical talks, and provided a very useful 'snapshot' of the state of electronic structure research in the field of superconductivity. It is clear that future progress will rely on methods which go beyond simple LDA/GGA functionals, and include both LDA+U approaches as well as realistic treatments of electron-phonon coupling.

### **Programme**

7 September 2009

Arrival and registration

8 September 2009

9.15, L. Boeri

10.00, P. Rourke

11.15 C. Bersier, JK Dewhurst and S. Sharma

14.30 S. Sanna

15.15 A. Borisenko

16.00 K. Wysokinski

9 September 2009

9.15, A. Floris

10.00, M. Calandra  
11.15 C. Ambrosch-Draxl  
14.30 R. Heid  
15.15 M. Putti  
16.00 short introductions to posters  
20.30 Poster session  
10 September 2009  
9.15, R. Gonelli  
10.00, G. Zwicknagl  
11.15 E. Perfetto  
14.30 A. Mackenzie  
15.15 Closing remarks  
18.15 musical evening with traditional sardinian instruments and voice

11 September 2009 Departure and optional excursion to The National Park of Asinara

### **Abstracts of presented papers**

Iron-based superconductors: what can we learn from DFT?  
L. Boeri, MPI-FKF Stuttgart, Germany

The discovery of superconductivity with a critical temperature  $T_c$  of 26 K in fluorine-doped LaOFeAs in early 2008 has initiated a so-called "iron age" in the field of superconductivity. In a few months, several new iron-based superconductors, with  $T_c$ 's as high as 55 K, have been found. Their crystal structures show a common motive, characterized by a square Fe lattice, surrounded by distorted tetrahedra of pnictogen or chalcogen atoms. Besides superconductivity, iron-based superconductors show a spin density wave (SDW) transition accompanied by a lattice distortion. This points to a possible unconventional origin of superconductivity, in analogy with the high- $T_c$  cuprates, although there is no general consensus on the pairing mechanism. In this talk, I will first review and discuss the main experimental findings concerning iron-based superconductors. I will then use Density Functional theory to describe the electronic and vibrational properties of LaOFeAs, which is a prototype compound for iron pnictides. Using linear response calculations, I will show that the standard Migdal-Eliashberg theory fails to account for the observed critical temperature.[1] Using an ab-initio effective tight-binding Hamiltonian, based on Fe d and As p Wannier orbitals, derived from NMTO downfolding, I will then analyze in detail the origin of the complicated band structure of iron pnictides, and use this tight-binding

model to discuss the origin of magnetism in Fe-based superconductors and its itinerant nature[2], which is probably at the basis of the observed failure of LDA in the description of their magnetic properties.[3].

[1] L. Boeri, O. V. Dolgov, and A. A. Golubov, Phys. Rev. Lett. 101, 026403 (2008) and cond mat/0902.0288.

2

O.K. Andersen and L. Boeri, in preparation.

3

I. I. Mazin, M. D. Johannes, L. Boeri, K. Koepernik, and D. J. Singh, Phys. Rev. B 78, 085104 (2008).

### **A transport perspective on scattering in the cuprates: the pseudogap, quantum criticality, and superconductivity**

P. Rourke, University of Bristol, UK

An overview of the Hussey group's recent work to unravel the temperature dependence, momentum dependence, and doping dependence of scattering in the high temperature cuprate superconductors, via magnetoresistance measurements. Our results point to an anisotropic scattering rate, with implications on possible pseudogap physics, quantum criticality, and superconductivity in these compounds.

### **Why magnetism in $\text{CeO}_{1-x}\text{F}_x\text{FeAs}$ and $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$ is different**

C. Bersier, JK Dewhurst and S. Sharma, Institut für Theoretische Physik, Freie University Berlin

Using state-of-the-art first-principles calculations we study the magnetic behaviour of  $\text{CeOFeAs}$ . We find the Ce layer moments oriented perpendicular to those of the Fe layers. An analysis of incommensurate magnetic structures reveals that the Ce-Ce magnetic coupling is rather weak with, however, a strong Fe-Ce coupling. Comparison of the origin of the tetragonal to orthorhombic structural distortion in  $\text{CeOFeAs}$  and  $\text{LaOFeAs}$  show marked differences; in  $\text{CeOFeAs}$  the distortion is stabilized by a lowering of spectral weight at the Fermi level, while in  $\text{LaOFeAs}$  by a reduction in magnetic frustration. Finally, we investigate the impact of electron doping upon  $\text{CeOFeAs}$  and show that while the ground state Fe moment remains largely unchanged by doping, the stability of magnetic order goes to zero at

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a doping that corresponds well to the vanishing of the Néel temperature.

**Competition of magnetism and superconductivity in high  $T_c$  superconductors: from cuprates to pnictides**

Samuele Sanna, Physics Department “A.Volta” University of Pavia, Pavia, ITALY

The recent discovery of the Fe-based superconductors open new chances to unravel the puzzle of the High  $T_c$  superconductivity. In particular the proximity between the superconducting and magnetic phases, like in cuprates, renovates the issue of whether they compete or cooperate to produce a high transition temperature. I will talk about the phenomenological behavior at the magnetic-superconducting crossover, where the two states often coexist nanoscopically. In particular, results from several  $\mu$ SR experiments on cuprates and pnictides will be discussed.

**ARPES of superconductors**

Sergey Borisenko, IFW-Dresden, Germany

I will overview our most recent results on high-temperature cuprate and pnictide superconductors as well as other density waves systems. The progress from the instrumental point of view will be demonstrated on the example of “1-cubed ARPES” end-station at BESSY which allows to collect photoemission data at temperatures below 1K.

**Orbital dependent pairing effects in  $\text{Sr}_2\text{RuO}_4$ : NMR relaxation rate**

Karol Wysokiski, Institute of Physics, M. Curie-Sklodowska University, Lublin, Poland

The p-wave chiral superconductor  $\text{Sr}_2\text{RuO}_4$  is a quasi-two dimensional, highly anisotropic system with three bands crossing the Fermi energy. Low temperature power law behaviour is observed in temperature dependent physical properties, including specific heat, penetration depth and NMR relaxation rate, which is consistent with the existence of a line of nodes in the quasiparticle gap. However the interpretation of these experiments is complicated by possible temperature dependencies arising from the multi-band or orbital dependent pairing. The calculations of the the NMR relaxation rate  $1/T_1$  on the basis of realistic orbital specific, three orbital, three dimensional model with phenomenological coupling constants will be presented. The model leads to the ground state with chiral - gapless order parameter on the  $\gamma$  sheet of the Fermi level and with nodes on the remaining two sheets.



Our results compare well with existing experimental  $^{101}\text{Ru}$  NQR data showing a relaxation rate  $1/T_1 \sim T^3$ , and no visible Hebel-Slichter like peak below  $T_c$ . On the other hand the diagonal  $d_{xy}$  orbital projected components of the relaxation rate show a more complex behaviour, including a Hebel-Slichter like peak below  $T_c$ . We speculate that these orbital dependencies might be related to the differences observed between spin relaxation rates for  $^{17}\text{O}$  and  $^{101}\text{Ru}$  nuclei in this material.

**Applications of density functional theory for the superconducting state** A. Floris, Institut für Theoretische Physik, Freie University Berlin

In this contribution we will review the basic theory of Superconducting Density Functional Theory (SCDFT) and some recent applications to some of the most relevant electron-phonon based superconductors, with particular emphasis to molecular hydrogen under high pressure.

**Origin of charge density wave behavior in bulk and few layers 2H-NbSe<sub>2</sub>** Matteo Calandra, Paris, France

We investigate the charge density wave (CDW) instability in 2H-NbSe<sub>2</sub> as a function of the number of layers. We demonstrate that density functional theory is able to describe the metallic charge density wave behaviour in bulk 2H-NbSe<sub>2</sub>. We predict that both bilayer and single-layer NbSe<sub>2</sub> undergo a CDW instability. However, while in the bilayer, as in the bulk, the instability occurs at momentum  $\mathbf{q}_{cdw} \approx \frac{2}{3}\mathbf{GM}$  and leads to a metallic state, in the single-layer occurs at  $\mathbf{q}_{cdw} \approx \frac{1}{4}\mathbf{GM}$  and leads to a semimetallic ground state, in agreement with recent experimental data. Finally we attribute the origin of the CDW behaviour to a large enhancement of the electron-phonon matrix element at momenta close to  $\mathbf{q}_{cdw}$ .

**Electron-phonon coupling in (un)conventional superconductors: the role of doping and its effect on the electronic structure** Claudia Ambrosch-Draxl Leoben, Austria

I will discuss the impact on electron-phonon coupling (EPC) on the electronic structure, the traces of which can clearly be seen in photoemission experiments. To this extent the GW approach is employed, solving the complex Dyson equation with the bare electronic bands as well as the Eliashberg function calculated from first principles. It will be shown that the EPC gives rise to complicated temperature-dependent band-splitting in the order of the phonon frequencies. This effect, which in general does not only show up

in superconductors, will be demonstrated for MgB<sub>2</sub>. To tackle the question of whether kinks seen in photoemission data of high-temperature superconductors are arising from the EPC, the phonon band structure of Ba doped La<sub>2</sub>CuO<sub>4</sub> is investigated. Here the strong correlations as well as structural phase transitions are challenging issues which need to be further explored before final conclusions can be drawn.

**Germany Electron-phonon coupling, self-energy effects and pairing interaction in YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> within the local density approximation.**

Rolf Heid, Forschungszentrum Karlsruhe, Institut für Festkörperphysik

Recent observations of kinks in the electronic dispersion and of phonon anomalies for several members of the cuprates have been suggestive of a strong interaction between electronic and lattice degrees of freedom in the high-T<sub>c</sub> superconductors. In this talk, I discuss a first principles study of the electron-phonon coupling in YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> in the framework of the local density approximation (LDA). Using a realistic phonon spectrum the momentum and frequency dependence of the coupling is calculated and its consequences for the electronic self-energy in the normal state and for the phonon-induced pairing interaction is analyzed. It is found that for electronic states close to the Fermi energy the phonon-induced self-energy is about a factor 5 too small compared to the experiment [1]. In addition, the phonon-induced pairing potential, relevant for superconductivity, exhibits a momentum dependence which is not favorable for pairing in the d-wave channel, leading to a coupling constant of only 0.022, which is even ten times smaller than the small value of the s-wave channel [2]. I will address implications for the above mentioned experimental observations as well as potential corrections due to strong correlations.

1

R. Heid, K.-P. Bohnen, R. Zeyher, D. Manske, Phys. Rev. Lett. **100**, 137001 (2008).

2

R. Heid, R. Zeyher, D. Manske, K.-P. Bohnen, Phys. Rev. B **100**, 024507 (2009).

**New Fe-based superconductor: huge upper critical fields, low coherence length, thermal fluctuation, paramagnetic limit**

Marina Putti , University di Genova, Italy

In 2008 the Hosono group discovered high temperature superconductivity in oxipnictide. After that several distinct families of superconductors (1111, 122, 11,111) based on Fe layers have been discovered. They share several characteristics with cuprate superconductors, like layered structure, small coherence length, non conventional pairing, that had been shown to make practical applications difficult, especially large thermal fluctuations. On the other hand pnictides are more metallic, anisotropy is generally smaller and does not strongly depend on the level of doping, the order parameter symmetry is supposed to be different. Despite the several similarities the different families exhibit important difference. The 1111 family, indeed, shows larger  $T_c$ , huge but also anisotropic upper critical field and in field fan-shaped resistive transition reminiscent of those of cuprates, while the 122 family is less anisotropic and presents sharper resistive transitions which are displaced in field like in low temperature superconductors. Finally 11 family has the lowest  $T_c$ , it is nearly isotropic, presents huge  $H_{c2}$  slope and not negligible thermal fluctuations. Upper critical field,  $H_{c2}$ , the electronic anisotropy parameter  $= H_{c2ab}/H_{c2c}$ , will be discussed and compared across the pnictide family.

**Point-contact Andreev-reflection spectroscopy in iron pnictides of the 1111 and 122 families: Evidence for two-gap nodeless superconductivity and strong electron-boson coupling** Renato S. Gonnelli, Dipartimento di Fisica and CNISM, Politecnico di Torino, Italy

The number, symmetry and amplitude of the gaps in the Fe-As superconductors are still open issues, as well as the origin of the electron pairing in these compounds. Here, we review our recent point-contact Andreev-reflection measurements in  $\text{SmFeAsO}_{0.8}\text{F}_{0.2}$  ( $T_c^{on}=53$  K) and  $\text{LaFeAsO}_{0.9}\text{F}_{0.1}$  ( $T_c^{on}=27$  K) polycrystals and present new results in  $\text{Ba}(\text{Fe}_{0.9}\text{Co}_{0.1})_2\text{As}_2$  single crystals. In all the cases, the low-temperature conductance curves clearly indicate the presence of two gaps in the superconducting state. No zero-bias peaks were observed, which rules out the d-wave symmetry. The gap amplitudes can be extracted from a generalized two-band BTK fit of the normalized conductance curves. The resulting values of the gaps,  $\Delta_1$  and  $\Delta_2$ , lie slightly below and well above the BCS value, respectively. In Sm-1111, their low-T values are  $\Delta_1(0) = 6.15 \pm 0.45$  meV and  $\Delta_2(0) = 18 \pm 3$  meV, which give gap ratios ( $2\Delta/k_B T_c$ ) of  $2.5 - 3$  and  $7 - 9$ , respectively. Both  $\Delta_1$  and  $\Delta_2$  show a BCS-like temperature dependence and close at the bulk  $T_c$ . In La-1111 we obtained similar gap ratios but the experimental situation is

more complex, depending also on the different local  $T_c$  shown by the contacts in crystallites with slightly different doping. At  $T_c$ , the normal-state conductance shows unusual features at zero bias (a depression in La-1111 and a hump in Sm-1111) that are progressively washed out on increasing temperature, to finally disappear at  $T^* \approx 140$  K, close to the Néel temperature of the parent compound. The experimental  $T_c$  and the gap values of the superconducting pnictides of both the families can be simultaneously reproduced within the Eliashberg theory by using a three-band model where the dominant role is played by interband interactions and the order parameter shows a  $s\pm$ -wave symmetry. High values of the electron-boson coupling constants and small typical boson energies (in agreement with experiments) are necessary to obtain the values of all the gaps and to correctly reproduce their temperature dependence. The presence of high-energy features (at  $E \approx \Delta_2$ ) in the conductance curves of  $\text{Ba}(\text{Fe}_{0.9}\text{Co}_{0.1})_2\text{As}_2$  single crystals, which can be related to a very strong electron-boson coupling is also presented and discussed.

Co-authors: D. Daghero, M. Tortello, G.A. Ummarino, V.A. Stepanov, J.S. Kim, R.K. Kremer, J. Karpinski, N.D. Zhigadlo and Jianyi Jiang

### **Layered organic metals: Novel superconducting states in high magnetic fields**

G. Zwicknagl, Braunschweig, Germany

Layered organic superconductors exhibit complex phase diagrams. Of particular interest is the fact that the upper critical fields separating normal and superconducting phases are unusually high. For field direction parallel to the conducting layers, they may exceed the estimated paramagnetic limit. In addition, there are indications for transitions between different superconducting states slightly below  $H_{c2}$ .

In this talk, I argue that the phase which separates the homogeneous superconducting state from the normal state is a realization of an inhomogeneous Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state. The latter arises due to the population imbalance of the paired fermions. I shall give a brief introduction into the quasiclassical theory of inhomogeneous superconductors which is adopted to calculate the critical fields using realistic band structure information. I shall discuss how electronic properties affect the formation and stability of the inhomogeneous superconducting states

### **Equilibrium and time-dependent Josephson currents in one-dimensional superconducting junctions** Enrico Perfetto, CNISM Roma "Tor Vergata"

We investigate the transport properties of a one-dimensional superconductor-normal metal- superconductor (S-N-S) system described within the tight-binding approximation. We compute the equilibrium dc Josephson current and the time-dependent oscillating current generated after the switch-on of a constant bias. In the first case an exact embedding procedure to calculate the Nambu-Gorkov Keldysh Green's function is employed and used to derive the continuum and bound states contributions to the dc current. A general formalism to obtain the Andreev bound states (ABS) of a normal chain connected to superconducting leads is also presented. We identify a regime in which all Josephson current is carried by the ABS and obtain an analytic formula for the current-phase relation in the limit of long chains. In the latter case the condition for perfect Andreev reflections is expressed in terms of the microscopic parameters of the model. When a finite bias is applied to the S-N-S junction we compute the exact time-evolution of the system by solving numerically the time-dependent Bogoliubov-deGennes equations. Our scheme allows us to describe the ac regime as well as the transient dynamics whose characteristic time-scale is dictated by the velocity of multiple Andreev reflections.

**Sr<sub>2</sub>RuO<sub>4</sub> and the physics of triplet pairing** Andy Mackenzie University of St Andrews, Scotland

In this talk I will review the body of experimental knowledge that has been accumulated about the unconventional superconductor Sr<sub>2</sub>RuO<sub>4</sub>, and then discuss a recent project in which the de Haas - van Alphen effect is being used to measure the influence of spin-orbit coupling on its Fermi surface.

**Orbital magnetic moment in a chiral p-wave superconductor**  
James Annett, University of Bristol, UK

The problem is the orbital angular momentum carried by the 3He A phase is a famous paradox. Naively a condensate of  $L_z=1$  hbar Cooper pairs will carry a corresponding macroscopic angular momentum, possibly entirely carried by a single chiral edge state. However in the case of the p-wave superconductor Sr<sub>2</sub>RuO<sub>4</sub> the condensate is also of  $L_z=1$  hbar Cooper pairs, and so should possess a finite ground state orbital magnetic moment. We discuss the calculation of this bulk moment in a realistic three band description of the superconductor, and compare our predicted moment with experiments including recent optical Kerr effect measurements. None

**Doping dependence of electron phonon interaction in La<sub>2-x</sub>Ba<sub>x</sub>CuO<sub>4</sub>**

Ali Tavana, University of Leoben (Austria) and Sharif University of Technology (Iran)

Density functional theory (DFT) calculations have been performed for the high-Tc superconductor  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$  (LBCO) in order to study the role of electron phonon (e-ph) interaction and lattice distortions. Using the virtual crystal approximation, calculations are performed for the entire doping range, i.e. for the undoped non-superconducting ( $x=0, 0.002$ ), for the superconducting ( $x=0.05, 0.075, 0.10$ ), for the overdoped region ( $x=0.20$ ), and for the “1/8 anomaly” ( $x=0.125$ ). The electronic ground states of LBCO for different Ba concentrations are also investigated using the LDA+U approximation to account for the strong electronic correlations. We study the interplay between antiferromagnetic (AF) order and nature of the ground state.

Phonon frequencies and e-ph interaction parameters  $\gamma(\mathbf{q}, \nu)$  are calculated based on the linear response theory. We find two degenerated strongly anharmonic phonon modes which soften around the M point and two other branches which exhibit softening around the Z point of Brillouin zone. Structural distortions related to those phonons are in accordance with the HTT to LTO and LTO to LTT phase transitions. We investigate the origin of the major contributions to the overall coupling parameter. The latter quantity is also analyzed in terms of the doping dependence. We discuss the results with respect to related experimental data.

**On the possible secondary component of the order parameter observed in London penetration depth measurements** Angelo Valli, Vienna University of Technology

Recent experiments show a low-temperature deviation from the pure d-wave behavior in the temperature dependence of the in-plane magnetic field penetration length in optimally doped  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_2$  and  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  compounds. This peculiar behaviour can reflect the presence of a secondary component of the superconducting order parameter, which has been proposed to be an isotropic s-wave. We show that a much more sensible description of the experimental results can be obtained assuming a time reversal breaking  $d_{x^2-y^2} + id_{xy}$  order parameters within a BCS approach for an effective low-energy model.

**Static and Dynamical Susceptibility of pure and doped LaOFeAs** Marco Monni, SLACS (INFN-CNR) and Department of Physics - University of Cagliari

The mechanism of superconductivity in pnictides is still under debate. The magnetic properties of these compounds suggest a possible role of spin fluctuations in the pairing mechanism. The effective interaction among electrons can be expressed in terms of the susceptibility  $\chi$ . The latter is therefore a key quantity in the determination of both the magnetic properties of the system in the normal state, and of the contribution of spin fluctuations to the pairing potential. A basic ingredient to obtain  $\chi$  is the independent-electron susceptibility  $\chi_0$ . Using  $\text{LaO}_{(1-x)}\text{F}_x\text{FeAs}$  as a prototype material, in this work we present a detailed ab-initio study of  $\chi_0$ , as a function of doping and of the internal atomic positions, starting from accurate electronic structures calculations within density functional theory.

**Magnetic properties of  $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$**  John Kay Dewhurst , Institut für Theoretische Physik , Freie University Berlin

Using state-of-the-art first-principles calculations we have elucidated the complex magnetic and structural dependence of  $\text{LaOFeAs}$  upon doping. Our key findings are that (i) doping results in an orthorhombic ground state and (ii) there is a commensurate to incommensurate transition in the magnetic structure between  $x = 0.025$  and  $x = 0.04$ . Our calculations further imply that in this system magnetic order persists up to the onset of superconductivity at the critical doping of  $x = 0.05$ . Finally, our investigations of the undoped parent compound reveal an unusually pronounced dependence of the magnetic moment on details of the exchange-correlation (xc) functional used in the calculation. However, for all choices of xc functional an orthorhombic structure is found.

**Scaling relations and virial theorems in density functional theory**  
Cesar R. Proetto, Freie Universitaet, Berlin

Scaling relations and virial theorems in density functional theory at thermodynamic equilibrium Scaling relations and virial theorems are derived for the relevant quantities of the density functional description of many-electron systems at thermodynamic equilibrium

Workshop Participants

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