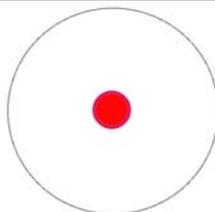
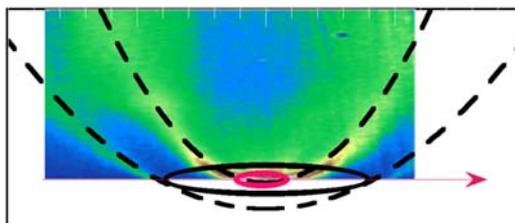

MULTI-CONDENSATES SUPERCONDUCTIVITY



edited by
Carlos Sa De Melo, Antonio Bianconi

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science series

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Superstripes 2014

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PREFACE

Multi-condensate superconductivity in different regions of either momentum space or real space is emerging as a common scenario for unconventional superconductivity found in novel complex materials discovered in the XXI century. Multi-band models with strong correlations to describe the low energy physics of Cuprate, Pnictide, Topological Superconductors and 2DEG Superconductivity at Interfaces are becoming increasingly necessary. Thus the purpose of this 2014 Erice summer school in solid state physics is to bring together scientist of different point of views to contribute for the critical assessment of existing knowledge in the field of this new fields of many different quantum macroscopic condensates in the process of emerging high temperature superconductivity. The top topic of this 2014 school is the low energy quantum many body physics of many different realizations of the scenario where the chemical potential is near a band edge.

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Abstracts

CHAPTER I

Interplay of disorder, nematicity and magnetism in Fe-based Superconductors

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Impurities can nucleate local magnetic states and give rise to quasi-long-range magnetic order in correlated electron systems. In the Fe-based superconductors, stripelike $(\pi,0)$ order usually prevails but competes with (π,π) antiferromagnetism. I show that in such a situation, unusual emergent defect states ("nematogens") can be created by nonmagnetic impurities which strongly break C_4 symmetry and may be responsible for local nematic defect structures observed by STM, as well as for the transport anisotropy observed in these materials.

Nematic Susceptibility in Systems with Magnetic, Orbital, and Lattice Degrees of Freedom

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Numerical measurements of the spin-nematic and orbital-nematic susceptibility as a function of the temperature for different values of the spin (orbital)-lattice coupling constant λ (g) were performed in order to reproduce and interpret the experimental measurements of the nematic susceptibility for iron pnictides.¹ A Ginzburg-Landau approach based on the numerical results was developed. It was found that within the spin-fermion model² with spin- and orbital-lattice couplings,³ the spin degree of freedom is the driver of the nematic and structural transitions. The numerical results indicate that the Néel temperature $T_N^{(0)}$ for the spin-fermion model uncoupled to the lattice defines the temperature $T^*=T_N^{(0)}$ that characterizes the temperature dependence of the spin-nematic susceptibility. It was observed that the structural and the nematic transition occur at a temperature $T_S > T^*$ which is a function of both g and λ . The spin-nematic susceptibility is fitted by $\chi_s = g/[a_0(T-T^*)+3T_S\psi^2]$ where ψ is the spin-nematic order parameter and a_0 is a constant both obtained numerically. For $T \geq T_S$ since ψ is very small the susceptibility is well fitted by the Curie-Weiss expression by $\chi_s = g/[a_0(T-T^*)]$. It was also observed that in the absence of coupling between orbital and magnetic degrees of freedom the orbital-nematic susceptibility is fitted by the expression $\chi_o = \lambda/(e_0+3f\Phi^2)$ where f is a parameter that depends on the couplings, e_0 is a constant and Φ is the orbital-nematic order parameter numerically determined. For $T \geq T_S$, $\chi_o = \lambda/e_0$ is a good fit for the data.

1. J._H. Chu et al., *Science* **337**, 710 (2012).
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3. S. Liang et al., *Phys. Rev. Lett.* **111**, 047004 (2013).

Shape Resonances in superconducting gaps in multi condensates superconductivity near a band edge

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Superconductivity in ultra-narrow superconducting units occurs in “heterostructures at atomic limit” [1,2] like boron, graphene, CuO₂, FeAs, FeSe layers and in synthetic nano-oxide-materials where a two dimensional electron gas (2DEG) is formed at the interface between two oxides. Here we show that an unconventional superconductivity at a BEC and BCS crossover occurs in the regime where two or more 2D or 1D bands cross the Fermi level forming multiple Fermi surface spots with different symmetry so that single electron hopping is forbidden while exchange-like interaction for pair transfer between the two condensates with different gaps is allowed [3-8]. This is the key ingredient of high temperature superconductivity where the shape resonance in the superconducting gaps appears by tuning the chemical potential near a band edge. Here the many body configuration interaction between the BCS-like condensate in the large Fermi surfaces and Bose-like condensate in the small Fermi surface gives origin to a particular case of Fano-Feshbach resonances in a particular BEC-BCS crossover. Here Fano meets Lifshitz in quantum condensates since at a metal-to-metal transition, where an additional Fermi surface with different symmetry appears by pressure or chemical doping, the configuration interaction of Fano scattering resonances meets the physics of the 2.5 Lifshitz transition where the chemical potential is tuned to a band edge [9]. We show the case of negative interference effects between the BCS and BEC condensates, typical of the Bose-Fermi models and negative U Hubbard models and the case for optimum superconducting regime where in the small Fermi surface a) the Fermi wavelength and the coherence length of the condensate are of the same order of magnitude and b) the pairing crosses from the antiadiabatic to adiabatic regime. We show that the key signature of Fano resonances in superconductivity gaps is the Fano anti-resonance dip in the gaps. The maximum critical temperature for material design is predicted where the chemical potential in the small Fermi surface is close to the Lifshitz critical point for “opening of a neck” at the crossover between a 1D to 2D topological transition of 2D-to-3D topological transition. Finally we discuss how scale free complex topology of Josephson junctions could favor the shape-resonances for the amplification of the critical temperature in complex superconducting networks of superconducting units [10-12]

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Type-1.5 superconductivity in multicomponent systems

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I will present theoretical arguments and discuss experimental evidence that some of the newly discovered multicomponent materials can have several coherence lengths and as a consequence of it have a different kind of superconductivity, which breaks the type-1/type-2 dichotomy. It was recently termed "type-1.5 superconductivity". This is a state where type-1 and type-2 flows are not antagonistic but coexistent, in particular resulting in long-range attractive, short-range repulsive intervortex interaction. In external field such a material can exhibit a macroscopic phase separation into vortex clusters and domains of Meissner state.

Competition between superconductivity and charge order in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$: A hard X-ray diffraction study

P Johan Chang¹, Elizabeth Blackburn², Alex Holmes², Markus Hucker³, Niels B. Christensen⁴, Jacob Larsen⁴, Ruixing Liang^{5,6}, Walter Hardy^{5,6}, Doug Bonn^{5,6}, Uta Rütt⁷, Olof Gutowski⁷, Martin von Zimmermann⁷, Ted Forgan², Stephen M. Hayden⁸,

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Recently, charge order has been probed by NMR [1], x-ray diffraction [2-5] and ultra sound [6] experiments in the cuprate system $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$. This talk presents, the most recent hard x-ray experiments [2-3] in high magnetic fields. The competition between charge order and superconductivity will be discussed.

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[2] E. Blackburn *et al.*, Physical Review Letters **110**, 137004 (2013)

[3] J. Chang *et al.*, Nature Physics **8**, 871 (2012)

[4] S. Blanco-Canosa *et al.*, Physical Review Letters **110**, 187001 (2013)

[5] G. Ghiringhelli *et al.*, Science **337**, 821 (2012)

[6] D. LeBoeuf *et al.*, Nature Physics **9**, 79 (2013)

Key words: High-temperature superconductivity, charge order, phase competition

Asymptotic scales in the spatial behaviour of two-gap superconductivity

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We have examined the properties of critical (diverging at the phase transition point) and non-critical (finite on the whole temperature scale) coherence lengths () in the framework of a two-band BCS-type model and a two-orbital negative- ξ_{\mp} Hubbard model with inter-band (inter-orbital) pair-transfer interaction. The lengths U determine (i) the variation of small incidental deviations from the homogeneous superconductivity background and (ii) the spatial dependencies of intra- and inter-band correlation functions for superconductivity fluctuations in the Gaussian approximation. The influence of a surface on superconductivity gaps in the case of large distances and the behaviour of gaps far from the centre of a vortex are also scaled by these characteristic lengths. However, the suppression of superconductivity near the surface as well as near the vortex centre involves the length-scales different from ξ_{\mp} . *The research was supported by the European Union through the European Regional Development Fund (Centre of Excellence "Mesosystems: Theory and Applications", TK114) and by the Estonian Science Foundation, Grant No 8991.*

Keywords: two-gap superconductivity, asymptotic length-scales, fluctuations

The relevant papers of the authors:

T. Örd, K. Rågo, A. Vargunin, *J. Supercond. Nov. Magn.* **25**, 1351 (2012).

G. Litak, T. Örd, K. Rågo, A. Vargunin, *Acta Physica Polonica A* **121**, 747 (2012).

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G. Litak, T. Örd, K. Rågo, A. Vargunin, *Phys. Stat. Sol. (b)*, DOI 10.1002/pssb.201349146, (2013).

High-Field Magnetotransport Studies of the Fermi Surface in the Electron-Doped Cuprate $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$

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Strong magnetic fields have recently proved to be a very powerful tool for probing the anomalous “normal state” of the high- T_c cuprate superconductors. An impressive example is a discovery of magnetic quantum oscillations (MQO) in a number of hole- and electron-doped cuprates, which provided essential information on their Fermi surfaces. By contrast to hole-doped cuprates, where MQO reveal a reconstructed Fermi surface in the underdoped regime, for the prototypical electron-doped compound $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ (NCCO) a reconstructed Fermi surface is found to persist in the overdoped regime, up to the highest superconducting doping level. Here we present a survey of high-field magnetotransport properties of high quality single crystals of NCCO, including magnetoresistance, Hall effect and magnetothermopower. The data allow us to trace the evolution of the two-band electronic structure throughout the superconducting doping range. In particular, they establish a remarkable correlation between the Fermi surface transformations and superconductivity in NCCO.

Keywords: cuprate superconductor; Fermi surface; magnetic quantum oscillations; magnetotransport

Multi-phase physics of multi-condensate superconductors

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U(1) rotational invariance is spontaneously broken in superconductors. The ground state has a long-range order by breaking the U(1) invariance and the massless Nambu-Goldstone boson exists. The Coulomb repulsive interaction turns the massless mode into a gapped plasma mode. In N-gap superconductors, the $U(1)^N$ phase invariance is spontaneously broken. This leads to multi-phase physics where additional phase invariance will bring about new excitation modes and novel phenomena.

In an N-gap superconductor, there are N-1 phase-difference modes. These modes are in general massive due to the Josephson interaction. We show that there are massless modes as well as massive modes when N is greater than 3. There are N-3 massless modes and two massive modes near the minimum of the Josephson potential when N bands are equivalent and Josephson couplings are frustrated. The global $U(1)^{N-1}$ symmetry is broken down by the Josephson term to $U(1)^{N-3}$.

We show that the phase-difference modes are interpreted as abelian gauge fields. A non-trivial topology of the gauge field is represented by a monopole singularity of the gauge field with the integer Chern number. This leads to a possibility of half-quantum flux vortices in a two-gap superconductor. A generalization to three-gap superconductors results in the existence of chiral states with time-reversal symmetry breaking and a fractionally quantized-flux vortex.

We also discuss fluctuation corrections of the Josephson interaction. The critical value of the coupling constant is determined by the renormalization group theory. This gives a characteristic temperature and number that indicate the fluctuation strength of phases of gap functions. We show that the characteristic temperature is in the same order as the Ginzburg temperature in two-space dimensions.

Mass Renormalizations and Unconventional Pairing in Superconducting Iron Pnictides

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Combining DFT calculations of the DOS and plasma frequencies with experimental thermodynamic and optical data, such as electronic specific heat and penetration depth, as well as available ARPES and dHvA data taken from the literature, we estimate both the high-energy (Coulomb, Hund's rule coupling) and low-energy (electron-boson coupling) electronic mass renormalization for several Fe-pnictides with $T_c < 40$ K, focusing on AFe_2As_2 ($A=K,Rb,Cs$), (Ca,Na)-122, (Ba,K)-122, LiFeAs, and $LaFeO_{1-x}F_xAs_{1-\delta}$ with and without As-vacancies. Using multiband Eliashberg theory, we show that these systems can NOT be described by a very strong el-boson coupling constant $\lambda \approx 2$ or even larger as often proposed in the literature, being in conflict with the significant high-energy mass renormalization as seen by ARPES and optics from one side and the total mass renormalization derived from available electronic specific heat data. Instead, an intermediately strong s_{\pm} -coupling regime is realized in high- T_c iron pnictides, essentially based on interband spin fluctuations from at least one predominant pair of bands. In some cases, e.g. $Ca_{0.32}Na_{0.68}Fe_2As_2$, there is also a non-negligible intraband el-phonon or el-orbital fluctuation contribution [1]. The coexistence of magnetic As-vacancies and high- T_c superconductivity excludes an s_{++} -scenario at least for $LaFeO_{1-x}F_xAs_{1-\delta}$. Difficulties of the standard DFT with respect to calculated and empirical partial DOS are discussed in terms of orbital dependent correlation effects.

[1] S. Johnston *et al.* Phys. Rev. B **89**, 134507 (2014).

Holographic Model of Two-Band Superconductor

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We construct a holographic two-band superconductor model with interband Josephson coupling. We investigate the effects of Josephson coupling to the superconducting condensates and critical temperature. We also compute the AC optical conductivity and thermal conductivity and find our model is nodeless

CHAPTER II

Monday – July 21st

Nature of magnetism and superconductivity in the three-dimensional electronic structures of Fe pnictides

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Interplay between magnetism, structural distortion, and superconductivity is the essential features of Fe-based superconductors. However, fundamental issues such as whether the magneto-structural transition is driven by Fermi-surface (FS) nesting or local magnetic moment formation and how important the FS nesting is for superconductivity have remained unclear. To resolve these issues, studies on systems with different structural parameters will give useful insight.

We have studied the FSs, band dispersions, and superconducting gaps of the $\text{BaFe}_2(\text{As,P})_2$ [1,2] and $\text{SrFe}_2(\text{As,P})_2$ [3] systems using ARPES. The T_N of the parent compound as well as the T_c of the optimally doped compound are higher in the $\text{SrFe}_2(\text{As,P})_2$ system than $\text{BaFe}_2(\text{As,P})_2$. Hole FSs are found to be more strongly warped in $\text{SrFe}_2(\text{As,P})_2$, suggesting that the magnetic ordering is not driven by FS nesting but by local moment formation, and interlayer magnetic interaction plays an important role. Mass renormalization is found to be stronger in $\text{SrFe}_2(\text{As,P})_2$, consistent with the stronger magnetism. The superconducting gap is more anisotropic for the electron and hole FSs in $\text{BaFe}_2(\text{As,P})_2$ and $\text{SrFe}_2(\text{As,P})_2$, respectively, that is, gap anisotropy and FS warping seem correlated.

This work has been done in collaboration with H. Suzuki, L. Liu, J. Xu, S. Ideta, T. Yoshida, K. Okazaki, T. Shimojima, Y. Ohta, S. Shin, M. Hashimoto, D. Lu, Z.-X. Shen, H. Anzai, A. Ino, M. Arita, H. Namatame, M. Taniguchi, H. Kumigashira, K. Ono, T. Kobayashi, S. Miyasaka, S. Tajima, S. Kasahara, T. Terashima, T. Shibauchi, Y. Matsuda, M. Nakajima, Y. Tomioka, T. Itoh, K. Kiho, C.-H. Lee, A. Iyo, H. Eisaki, and S. Uchida.

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[2] T. Yoshida et al., *arXiv:1301.4818*.

[3] H. Suzuki et al., *arXiv:1312.4687*.

Keywords: Fe-based superconductors, magneto-structural transition, superconducting gap

ARPES study on FeSe/STO and FeSe/BTO films

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The record of superconducting transition temperature (T_c) has long been 56 K for the iron-based high temperature superconductors (Fe-HTS's). Recently, in single layer FeSe films grown on SrTiO₃ substrate, signs for a new 65 K T_c record are reported. Combining molecular beam epitaxy and *in situ* angle resolved photoemission spectroscopy (ARPES), we study the ultra thin FeSe films on various substrates. We substantiate the presence of spin density wave (SDW) in FeSe films, a key ingredient of Fe-HTS that was missed in FeSe before, which weakens with increased thickness or reduced strain. We demonstrate that the superconductivity occurs when the electrons transferred from the oxygen-vacant substrate suppress the otherwise most pronounced SDW in single layer FeSe. We establish the phase diagram of FeSe vs. lattice constant that contains all the essential physics of Fe-HTS's [1]. With first principle calculations, we show that the superexchange interactions across Fe-As-Fe is enhanced with increased lattice constant [2].

By fabricating FeSe/STO/KTO hetero-structure, we further enhanced the lattice constant of FeSe, and increased the gap-closing temperature to 70K. Two unhybridized electron Fermi surfaces are resolved, and the superconducting gap exhibits strong anisotropy around the individual Fermi surface. This observation ruled out many existing theories on the pairing symmetry of iron chalcogenide superconductors with only electron pockets [3].

By fabricating FeSe/BTO/KTO hetero-structure, we further enhance the gap-closing temperature to 75K. We show that the interface has a highly nontrivial role on the electron correlation, and superconductivity [4].

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Keywords: *interfacial superconductivity, ARPES, iron-based superconductors*

Non-Equilibrium momentum dependent dynamic of high temperature superconductors

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In this talk I will present an overview of Time- and Angle- Resolved Photoemission spectroscopy studies on high temperature cuprate superconductors.

The effects of optical excitation on the electronic structure and study of the resulting quasiparticles, superconducting gap, and Cooper pair formation dynamics near their natural time- scales are discussed. Direct measurements of these and other non-equilibrium spectral phenomena through the phase diagram further illustrate the power of this technique and reveal a new window into the nature of the pairing interaction in high T_c superconductors.

Band-edge BCS-BEC crossover in a two-band superconductor: physical properties and detection parameters

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Superconductivity in iron-based, magnesium diborides, and other novel superconducting materials has a strong multi-band and multi-gap character [1] and recent experimental evidences support the possibility for a BCS-BEC crossover induced by strong-coupling and proximity of the chemical potential to the band edge of one of the bands [2, 3]. Here we study the simplest theoretical model which accounts for the BCS-BEC crossover in a two-band superconductor, considering tunable interactions and different energy separations between the bands. Mean-field results for the condensate fraction, the correlation length, and the superconducting gaps are reported in typical crossover diagrams to locate the boundaries of the different BCS, crossover and BEC regimes when the band edge is approached. When the superconducting gap is of the order of the local chemical potential, superconductivity is in the crossover regime of the BCS-BEC crossover and the Fermi surface of the small band is completely smeared by the gap opening. In this situation, small and large Cooper pairs coexist in the total condensate, which is the optimal condition for high-T_c superconductivity [4]. The ratio between the gap and the Fermi energy in a given band results to be the best detection parameter for experiments to locate the system in the BCS-BEC crossover. Using available experimental data, our analysis shows that iron-based superconductors have the partial condensate of the small Fermi surface which is in the crossover regime of the BCS-BEC crossover [5], supporting in this way the recent ARPES findings [6, 7].

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Charge-Orbital-Spin Multimode Fluctuations due to Vertex Correction in Fe-Based Superconductors, High- T_c Cuprates, and Ruthenide

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In the iron-based superconductors, the evidences of orbital order and fluctuations have been accumulated. Recently, we have shown that strong orbital and spin fluctuations mutually develop in multiorbital systems due to the vertex correction (VCs), which is dropped in the mean-field approximations [1-6]. In Ref.[2], we study the phase diagram of $\text{LaFeAsO}_{1-x}\text{H}_x$, in which the isostructural (C_4) transition is realized at $x\sim 0.5$, in addition to the conventional orthorhombic (C_2) structure transition at $x\sim 0$. It is found that the trigger of the C_4 (C_2) structure transition is the non-nematic (nematic) orbital order [1,3]. We also study the gap structure in LiFeAs , which is an important “fingerprint” of the pairing mechanism. The absence of the nesting in LiFeAs attracts great attention. The largest gap is realized on the tiny hole-pockets composed of d_{xz}, d_{yz} orbitals. This fact is naturally explained in terms of the orbital-fluctuation-mediated superconductivity, due to the better inter-orbital nesting of LiFeAs .

The VC plays important roles in other multiorbital systems. We show that the orbital order/fluctuations due to the VC give rise to the “electronic nematic order” in $\text{Sr}_3\text{Ru}_2\text{O}_7$ [4], the “spin-triplet superconductivity” in Sr_2RuO_4 [5], and the “CDW order at $Q\sim(0.25,0)$ ” with interorbital charge transfer in cuprates [6]: The predicted charge pattern is very similar to the STM results. We predict that the strong charge-orbital-spin mode-coupling due to VC gives the multimode fluctuations in Fe-pnictides, cuprates, and ruthenides, which will be ubiquitous in strongly correlated systems.

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Key Words: Fe-based superconductors, ruthenates, cuprates, vertex correction

Superconductivity from repulsion in multiband layered systems: novel s-wave symmetry in LiFeAs and possible symmetries in BiS₂ superconductors

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In my talk we will review the multiband aspects of superconductivity arising from repulsive interaction with weak spin fluctuations. Most importantly, I will analyze the structure of the pairing interaction and superconducting gaps for LiFeAs, which electronic structure and superconducting gaps are well studied by ARPES. We use the ten-orbital tight-binding model, derived from ab-initio LDA calculations with hopping parameters extracted from the fit to ARPES experiments. We find that the pairing interaction almost decouples between two subsets, one consists of the outer hole pocket and two electron pockets, which are quasi-2D and are made

largely out of dxy orbital, and the other consists of the two inner hole pockets, which are quasi-3D and are made mostly out of dxz and dyz orbitals. Furthermore, the bare inter-pocket and intra-pocket interactions within each subset are nearly equal. In this situation, small changes in the intra-pocket and inter-pocket interactions due to renormalizations by high-energy fermions give rise to a variety of different gap structures. Different s-wave gap configurations emerge depending on whether the renormalized interactions increase attraction within each subset or increase the coupling between particular components of the two subsets. We argue that the state with opposite sign of the gaps on the two inner hole pockets has the best overlap with ARPES data.

In the second part of my talk I will analyze the realistic minimal electronic model for recently discovered BiS₂ superconductors including the spin-orbit coupling based on a first-principles band structure calculations. Due to strong spin-orbit coupling, characteristic for the Bi-based systems, the tight-binding low-energy model necessarily includes p_x, p_y, and p_z orbitals. We analyze a potential Cooper-pairing instability from purely repulsive interaction for small and intermediate doping concentrations and find d-wave, and s₊₋-wave symmetries, respectively, to be the dominant symmetries. Quasiparticle interference and spin response can be used to determine the symmetry of the order parameter in these systems.

Pauli-Limiting Effects in Multiband Iron-Pnictide Superconductors

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Spin-singlet superconductivity can be suppressed via the application of a magnetic field by two well-known mechanisms: orbital pair-breaking occurs when the charge-carrier motion is forced into cyclotron orbits, and Pauli or paramagnetic pair-breaking, when the quasiparticles are polarized by Zeeman-splitting, forcing the superconducting state to be suppressed via a first-order phase transition [1]. Pauli-limiting effects become important when the orbital shielding currents are reduced due to low-dimensional electronic structures. A challenging issue is the possibility of strong Pauli-limiting effects in multiband superconductors [2], in which bands contributing to the Fermi-surface might have different dimensionality, and thus the condition for a discontinuous phase transition might differ from band to band [3]. For example, in the iron-pnictide $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}$ series, increasing the K content lowers the dimensionality of the electronic structure and gives rise to strong correlations. These conditions favor Pauli pair-breaking effects in KFe_2As_2 , where we found compelling evidence for Pauli-limited multiband superconductivity [4]. In more general terms, our experiments have shown the complex interplay of pair breaking and multiband effects, which have to be taken into account in models of multiband superconductivity in iron-based superconductors.

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Thermodynamics and Multiband Effects in Iron Pnictide Superconductors

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We report an exhaustive thermodynamic study (heat capacity, magnetization, thermal expansion) of the normal- and superconducting-state properties of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ high-quality single crystals ($x = 0 - 1.0$). The existence of strong correlations that develop with increasing hole concentration give evidence of the possible proximity to an orbital-selective Mott transition. In the superconducting state, strong multiband and paramagnetic effects are observed and we bring evidence of a strong-to-weak-coupling crossover that occur near the concentration where the electron sheets disappear. Our data show no evidence for a symmetry change, from s to d -wave, of the superconducting state. Dissimilarities with the $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ series are emphasized.

Superconductivity in doped bismuth selenide

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Bismuth selenide is a topological insulator with topologically protected metallic surface states that exhibit a Dirac-like dispersion. The unique properties of these states offer possibilities for use in quantum information applications, such as creating and observing Majorana fermions, but these applications require interfaces with superconductors. Native bismuth selenide is a layered compound with weak van der Waals couplings between the layers - by intercalating metal atoms between the layers, bismuth selenide can be made superconducting. I will describe our recent measurements of resistance as a function of temperature and magnetic field in Pd-doped bismuth selenide. Depending on the level of doping, we observe either partial or full superconducting transition, with an unusual subgap structure. I will discuss the origin and the nature of superconductivity in this doped topological insulator.

Phase Diagram and High Temperature Superconductivity at 65K in the Single-Layer FeSe Films Revealed by ARPES

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The discovery of the iron-based superconductors in 2008 not only provides another venue to understand the origin of high-T_c superconductivity but also a new playground to explore novel superconductors with higher superconducting transition temperature. The latest report of possible high temperature superconductivity in the single-layer FeSe films grown on SrTiO₃ substrate is both surprising and interesting [1]. In this talk, we report the electronic structure and phase diagram of the single-layer FeSe films by angle-resolved photoemission spectroscopy (ARPES) [2,3]. Our high-resolution ARPES results show that it has a simple Fermi surface topology consisting only of electron pockets near the zone corner without indication of any Fermi surface around the zone center. In addition, our observation of large and nearly isotropic superconducting gap in this strictly two-dimensional system rules out existence of node in the superconducting gap. We also established a phase diagram in this single-layer FeSe films by an annealing procedure to tune the charge carrier concentration over a wide range. By optimizing the annealing process, we observed evidence of a record high T_c of ~65K in the single-layer FeSe films. The wide tunability of the system across different phases, and its high-T_c, make the single-layer FeSe film ideal not only to investigate the superconductivity physics and mechanism, but also to study novel quantum phenomena and for potential applications.

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CHAPTER III

Tuesday – July 22nd

Evolution of two-band superconductivity from weak (BCS) to strong (BEC) coupling

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In this lecture, I review some key points regarding the evolution of two-band superconductivity from the weak to the strong coupling (Bardeen Cooper Schrieffer to Bose Einstein condensation) regimes [1-3]. I also describe how population imbalances between the two bands can be created by tuning the intraband or interband (Josephson) interactions. When the Josephson interband interaction is tuned from negative to positive values, a quantum phase transition occurs from a 0-phase to a π -phase state, depending on the relative phase of the two order parameters. In addition, I describe two undamped low energy collective excitations corresponding to in-phase phonon (Goldstone) and out-of-phase exciton (finite frequency) modes. Furthermore, I describe the emergence of coupled Ginzburg-Landau equations, and show that they reduce to coupled Gross-Pitaevskii equations for two types of weakly interacting bosons (tightly bound fermions) in the BEC limit. Lastly, I comment on new theoretical developments in this area from my group [4].

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Nanoscale superconductors: influence of quantum confinement

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It is well known that when the dimensions of a superconductor are comparable to the Fermi wavelength, the superconducting properties will be strongly affected by quantum confinement. For example, shape resonances appear and manifest as oscillations of the critical temperature with the lateral dimension. By numerically solving the Bogolibov-de Gennes equations, we uncover several peculiar effects induced by quantum confinement. First we show that the vortex structure of a nanoscale superconducting square deviates from the conventional structure observed at mesoscopic scales, and is dependent on the ratio between superconducting coherence length and the Fermi wavelength[1]. We found a plethora of unconventional vortex ground states and the tendency of forming multi-vortex rather than giant-vortex configurations[2]. Next we present the effect of non-magnetic impurities and show that: 1) impurities strongly affect the superconducting properties, 2) the effect is impurity position-dependent, and 3) it exhibits opposite behavior for resonant and off-resonant wire widths [3].

** Work done in collaboration with L.F. Zhang, L. Covaci, G.R. Berdiyrov and M.V. Milosevic.*

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Selective Mottness as a key to iron superconductors

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The phase diagram of the high- T_c cuprates is dominated by the Mott insulating phase of the parent compounds. As we approach it from large doping, a standard Fermi-liquid gradually turns into a bad non-Fermi liquid metal, a process which culminates in the pseudogap regime, in which the antinodal region in momentum space acquire a gap before reaching a fully gapped Mott state. The strong correlation effects are therefore believed to be the unifying element to understand both the anomalous normal state and the superconducting phase.

On the other hand, in iron-based superconductors the parent compounds are not Mott insulators, and the role of electron correlations is still unclear and debated.

Here we show that experiments for electron- and hole-doped BaFe_2As_2 support indeed a scenario very similar to that of the cuprates. The doping evolution of the effective mass is dominated by the influence of a Mott insulator that would be realized for half-filled conduction bands, while the metallic stoichiometric compound does not play a special role. Weakly and strongly correlated conduction electrons coexist in much of the phase diagram, an effect which increases with hole doping.

We identify the reason for this behavior in a strong Hund's coupling, which decouples the different orbitals. Each orbital then behaves as an independent doped Mott insulator, where the correlation degree only depends on how doped is each orbital from half-filling.

Our scenario reconciles contrasting evidences on the electronic correlation strength and establishes a deep connection with the cuprates.

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Keywords: Iron-Superconductors, Selective Mottness, Hund's coupling

Itinerant multi-orbital models for Pnictide Superconductors

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Since several bands cross the Fermi surface of iron-based superconductors, an orbital degree of freedom becomes relevant, and orbital effects have been suggested as an explanation of the strongly anisotropic properties of the undoped parent compounds, and are also proposed as an explanation for 'accidental' nodes. However, the itinerant character of pnictides also leads to substantial differences compared to orbital order as it has been extensively discussed in Mott insulators. We apply numerical techniques to itinerant multi-orbital models in order to investigate magnetic and orbital order as well as their interplay. While the orbital character of the electrons at the Fermi surface is strongly affected by the magnetic order, the differences total densities in various orbitals turn out to be less crucial for low-energy properties. Concerning a phase with broken rotational symmetry, orbital-order and spin-nematicity driven scenarios are compared.

Exploration of (Fe, Ni)-Chalcogenide superconductors: Fe-vacancy order, new AFM ground state and Superconductivity

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Cuprates and Fe-based compounds are two families with highest superconducting (SC) transition temperatures. A common feature in both families is that the superconductivity emerges as antiferromagnetic (AFM) long range order is suppressed. While the parent compound of cuprates is a Mott insulator where the electron repulsion is strong, the parent compound of Fe-based materials is metallic implying weak or moderate electron correlation. A key strategy to develop a unified picture for the Fe- and Cu-based high temperature superconductivity (HTSC) is to explore the possibility to tune the Fe-based compound into an insulator. The relationship between the antiferromagnetic ground state in the Fe-chalcogenides, which is different from that in the Fe-pnictides, and superconductivity is another issue.

Here, firstly, I shall talk about the discovery of superconductivity with $T_C=14\text{K}$, determining of the lattice, magnetic structures in the parent of Fe(Te,Se,S) system and the correlation between bi-collinear AFM order and superconductivity in this system. Secondly, I shall discuss about our efforts on searching for new Fe-Chalcogenides with AFM insulating behavior, such as $\text{La}_2\text{O}_3\text{Fe}_2(\text{Se,S})_2$ compounds. Thirdly, I shall report our discovery of superconductivity above 30K in $(\text{Tl,K,Rb})\text{Fe}_x\text{Se}_2$ system, which the onset SC transition temperature is as high as 40K. While the compound with more Fe vacancies shows an AFM insulator behavior, which may be associated with the Fe-vacancy ordering in the crystals. Our discovery represents the first Fe-based HTSC at the verge of an AFM insulator. A review on the results of Fe-vacancy super-lattice, magnetism and superconductivity in $(\text{Tl, K, Rb})\text{Fe}_x\text{Se}_2$ system will be presented in this talk. Finally, I shall talk about the magnetism and superconductivity, discovered recently by us, in the $\text{TiNi}_2(\text{Se,S})_2$ and their doped compounds. A review on the new results of AFM order and superconductivity in their doped system will also be presented in this talk.

Infrared spectroscopic studies of iron-based superconductors

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The optical properties of $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ have been determined in the normal state for a number of temperatures over a wide frequency range. Two Drude terms, representing two groups of carriers with different scattering rates ($1/\tau$), well describe the real part of the optical conductivity $\sigma_1(\omega)$. A “broad” Drude component results in an incoherent background with a T-independent $1/\tau_b$, while a “narrow” Drude component reveals a T-linear $1/\tau_n$, resulting in a resistivity $\rho_n = 1/\sigma_{1n}(\omega \rightarrow 0)$ also linear in temperature. An $\arctan(T)$ low-frequency spectral weight is also strong evidence for a T-linear $1/\tau$. A comparison to other materials with similar behavior suggests that the T-linear $1/\tau_n$ and ρ_n in $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ originate from scattering from spin fluctuations and hence that an antiferromagnetic quantum critical point is likely to exist in the superconducting dome.

CHAPTER IV

Wednesday – July 23rd

Unconventional superconductivity and its intertwined phases

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Unconventional superconductivity (SC) is said to occur when Cooper pair formation is dominated by repulsive electron–electron interactions, so that the symmetry of the pair wave function is other than an isotropic s-wave. The strong, on-site, repulsive electron–electron interactions that are the proximate cause of such SC are more typically drivers of commensurate magnetism. Indeed, it is the suppression of commensurate antiferromagnetism that usually allows this type of unconventional superconductivity to emerge. Importantly, however, intervening between these AF and SC phases, intertwined electronic ordered phases of an unexpected nature are frequently discovered. For this reason, it has been extremely difficult to distinguish the microscopic essence of the correlated superconductivity from the often spectacular phenomenology of the intertwined phases. In this talk I introduce a model conceptual framework within which to understand the relationship between the antiferromagnetic electron–electron interactions, the intertwined phases, and correlated superconductivity. I demonstrate its effectiveness in simultaneously explaining the consequences of AF interactions for the copper-based, iron-based, and heavy-fermion superconductors, as well as for their quite distinct intertwined phases."

Spin fluctuations and high-temperature superconductivity in cuprates

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A microscopic theory of spin excitations and superconductivity in systems with strong electron correlations as cuprates is presented. An exact representation for the dynamic spin susceptibility in the normal and superconducting states within the t - J model is derived [1]. The spectrum of spin excitations is studied in a broad region of doping and temperature. A magnetic resonance mode in the superconducting and undoped normal phase is found which is weakly depends on temperature as observed in experiments.

Electronic spectrum and superconductivity are studied in the limit of strong correlations within the extended Hubbard model where the intersite Coulomb repulsion V and electron-phonon interaction are taken into account [2]. Both a weak and strong Coulomb repulsion V is considered. The Dyson equation for the normal and pair Green functions expressed in terms of the Hubbard operators is derived. We found the d -wave pairing with high- T_c mediated by spin fluctuations induced by strong kinematic interaction for the Hubbard operators of the order of kinetic energy of electrons $W \sim 2$ eV. Contributions to the d -wave pairing coming from a realistic in cuprates intersite Coulomb repulsion and phonons turned out to be small. Superconductivity can be suppressed only for large $V > W$.

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Keywords: *strong electron correlations, spin excitations, superconductivity, cuprates*

Electromagnetic response of strongly disordered superconductors

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In the last decades the failure of the BCS paradigm of superconductivity in several correlated materials led to a profound modification of the description of the superconducting phenomenon itself. A case in point is the occurrence of Cooper pairing and phase coherence at distinct temperatures, associated respectively with the appearance of a single-particle gap and a non-zero superfluid stiffness. This particular behavior is observed in several materials, which range from high-temperature cuprate superconductors to strongly-disordered films of conventional superconductors. For the latter systems scanning tunneling microscopy measurements have revealed that the superconducting state becomes inhomogeneous, segregating into domains of large and suppressed superconducting order parameter. In this talk we will discuss the electromagnetic response of such systems based on studies of the attractive Hubbard model with strong on-site disorder. Static and dynamical properties of current correlations are investigated by including fluctuations beyond the Bogoljubov-de Gennes approach.

In the static limit we find a strong renormalization of the superfluid stiffness due to the occurrence of quasi one-dimensional percolative current patterns which connect superconducting islands. Moreover we show that for strongly disordered superconductors phase modes acquire a dipole moment and appear as a subgap spectral feature in the optical conductivity.

Keywords: disordered superconductors, electromagnetic response, attractive Hubbard model

Variational investigation of superconductivity in two-dimensional Hubbard models

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Gutzwiller wave functions have been used extensively in the past 40 years for the study of correlated electron systems. In most applications, these wave functions have been evaluated by means of the 'Gutzwiller approximation' which becomes exact in the limit of infinite dimensions. For the study of correlation-induced superconductivity in finite-dimensional systems, however, one needs to improve this approximation. This can be achieved by a diagrammatic expansion which will be explained in detail in this presentation [1]. It has allowed us to study superconductivity or nematic ('Pomeranchuk') order in two-dimensional Hubbard [2] and t-J models [3]. Due to the numerical efficiency of the approach the study of multi-orbital systems is also feasible.

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Topologically stable gapped state in a layered superconductor

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An important concept in condensed matter physics is that of an order parameter, introduced by Lev Landau in the last century to describe the transition to the superconducting state. Interestingly, one of Landau's first proposals of an order parameter was the supercurrent, also suggested to exist in the microscopic superconducting ground state of Felix Bloch. These ideas were soon dismissed since a spontaneous circulating supercurrent increases the kinetic energy. Nevertheless an excited but stable state with spontaneously circulating supercurrents is possible and we find one containing flow and counter flow even without the presence of an external magnetic field. This is a skyrmion state found to exist above the homogeneous state in a layered superconductor, described by a two-component order parameter. The decay of the skyrmion state into other configurations of lower free energy is prevented by its topological stability, which gives rise to an energy gap. The skyrmion state breaks the time reversal symmetry and produces a very weak magnetic field inside the superconductor due to the supercurrents. The gap above the ground state, the topological stability and the unusual magnetic order that breaks the time reversal symmetry leads us to suggest that the pseudogap of the layered superconductors is indeed a skyrmion state [1, 2].

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Multicondensate Superconductivity in a Generalized BEC Formalism

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A recent attempt [1]-[3] to better understand the Bardeen-Cooper-Schrieffer (BCS) theory in terms of a *ternary* boson-fermion (BF) model is sketched. This ternary model contrasts with the more familiar *binary* models of, e.g., Eagles, Ranninger, Micnas, Robaszkiewicz, T.D. Lee, etc. The fermions are unpaired electrons (e) or, without loss of generality, holes (h); the bosons are Cooper pairs (CPs) of both these fermions. In essence, this statistical model, as BCS, gives a new generalized Bose-Einstein condensation (GBEC) formalism yielding *three* condensed chemically- and thermodynamically-stable phases: two pure BEC phases, one for 2e-CPs and one for 2h-CPs, along with a mixed phase in arbitrary proportions of each of the two pure phases. Besides including as special cases all known statistical models of superconductors the GBEC formalism leads to substantial enhancements [5], compared with BCS theory in the critical superconducting temperature. Lastly, with a binary model alone (i.e., no hole pairs) one can qualitatively show [6]-[8] how superconductor gaps, pseudogaps, domes, and “Fermi arcs” result in high-temperature superconducting cuprates, again with an ordinary BCS model interaction mimicking coulombic repulsions overwhelmed by electron-phonon attractions.

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Fingerprints of Spin-Orbital Entanglement in Transition Metal Oxides

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Spin-orbital superexchange models describe the low-energy degrees of freedom in Mott insulators and are in general characterized by entangled states [1]. They provide a theoretical framework for describing magnetic and optical properties of Mott insulators [2]. Several examples of spin-orbital models with highly anisotropic and intrinsically frustrated interactions are discussed. Spin-orbital entanglement concerns in general not only ground but also excited states and is observed, for instance, in several properties of the RVO_3 perovskites ($R=La, \dots, Lu$) at finite temperature, including the phase diagram [3], with phase transitions to orbital and spin order. We suggest that spin-orbital entanglement can be experimentally explored by the measurement of the dynamical spin-orbital correlations using resonant inelastic x-ray scattering. Spin-orbital entanglement is also responsible for noncollinear exotic magnetic antiferromagnetic order in the two-dimensional Kugel-Khomskii model [4]. Finally, on the example of the exactly solvable $SU(2) \times XY$ chain we show that changing the topology from an open to a periodic chain reduced the degeneracy of the ground state and enhances spin-orbital entanglement [5]. This novel type of topological order emerges from changing the chain topology and is reminiscent of the infinite- U Hubbard chain.

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Keywords: superexchange, spin and orbital order, phase transition, spin-orbital entanglement

New developments in superconductivity at high magnetic fields

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Here, I will discuss high magnetic field results [1, 2] in the superconducting state of URu₂Si₂, which was claimed to be a candidate for a chiral *d*-wave superconductor having a $k_z(k_x+ik_y)$ pairing symmetry. Through low temperature torque magnetometry, we show that the diamagnetic signal expected from vortex pinning, crosses over to an enhanced paramagnetic-like response for fields just below H_{c2} when the field approaches the ab-plane. We argue that this anomalous response can only be attributed to supercurrents circulating in the opposite sense with respect to the screening supercurrents, and therefore it might correspond to possible evidence for the sought after chiral state. Remarkably, we have seen a similar response also in LiFeAs [3, 4]. For both compounds, only the highest quality single crystals (i.e. lowest residual resistivity) are found to display such an effect, suggesting superconducting states that are very sensitive to disorder. We will also discuss the observation, through the de Haas van Alphen effect, of small nearly isotropic Fermi surface sheets in LiFeAs [4]. Finally, we will briefly discuss the properties of new Pd based chalcogenide superconductors displaying extremely high upper critical fields [5, 6].

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Keywords: chiral superconductivity, de Haas van Alphen, transition metal chalcogenide superconductors

CHAPTER V

Thursday – July 24th

Charge order, Fermi-arc instability, and d-wave bond-order in underdoped cuprates

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Charge-ordered (CO) ground states permeate the phenomenology of 3d-based transition metal oxides, and more generally represent a distinctive hallmark of strongly-correlated states of matter. The recent discovery of CO in various cuprate families fueled new interest into the role played by this incipient broken symmetry within the complex phase diagram of high-T_c superconductors. In our work, we investigate the origin and characteristics of CO states in single- (Bi2201) and bi-layer (YBCO) compounds, using a suite of complementary real- and momentum-space, and surface and bulk probes – resonant X-ray scattering (REXS), scanning-tunneling microscopy (STM), and angle-resolved photoemission spectroscopy (ARPES). By bringing together these techniques on Bi2201, we identify the connection between CO and the Fermi arcs to occur via the hot spots, and detect a charge modulation onset right below T* – thus pointing to an intimate relationship between the coexisting CO and PG orders [1].

In addition, we have also explored the local symmetry of charge modulations, and reveal it to correspond to a d-wave bond order [2]. The commonality between the symmetry of the order parameter for superconductivity and CO suggests that the same attractive interaction responsible for particle-particle (Cooper) pairing might also be active in the particle-hole channel.

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Triplet Pairing Superconductivity in Sr₂RuO₄

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The 1.5K superconductor Sr₂RuO₄ was discovered twenty years ago in 1994[1]. It remains very interesting because it is one of the best studied materials which may exhibit spin triplet superconductivity. A number of experiments strongly suggest this pairing state, including strong sensitivity to non-magnetic disorder, Knight shift, and phase sensitive tunnelling experiments. In particular both muon spin rotation and optical Kerr effect measurements imply a time reversal symmetry broken ground state, analogous to the ABM state of superfluid 3-He. However there still remain important unanswered questions: in particular the nodal structure of the gap function and the orientation of the spin triplet d-vector (in or out of plane) and its field dependence. Experimentally superconductivity seems to exist on all three Fermi surface sheets, but it remains an important open question which of these is dominant and provides the dominant pairing interaction leading to the superconductivity. In this talk I will review the recent experimental and theoretical studies of this material.

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Keywords unconventional superconductivity, triplet pairing, time reversal symmetry breaking

Optical Kerr effect in the chiral three band superconductor Sr_2RuO_4

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Strontium ruthenate is an interesting system with Fermi liquid like normal state at low temperatures and very anomalous superconducting state. It has been proposed that it is spin triplet odd parity superconductor. The proper interpretation of the experiments is challenging in many ways. The superconducting state of this tetragonal system breaks time reversal symmetry which points to the chiral state allowed by the group-theoretical analysis, its thermodynamic properties showing power low temperature dependence at low T require gap which vanishes somewhere at the Fermi surface. Such a state is not consistent with triplet pairing and tetragonal symmetry. The T independent spin susceptibilities measured with a magnetic field in a *ab* plane and along *c*-axis are at odds with the theory which require one of components to change with temperature. Also the Kerr effect in the chiral triplet superconductor Sr_2RuO_4 has proved difficult to explain unless either impurity scattering or multiband superconductivity are included in the theory. During the talk I will concentrate on the analysis of the ac Hall conductivity $\sigma_H(\omega)$ and the Kerr signal in terms of a realistic three dimensional three band model of the Fermi surface.

(in collaboration with James Annett and Martin Gradhand, University of Bristol)

Optical Birefringence and Dichroism of Cuprate Superconductors in the THz regime

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The presence of optical polarization anisotropies, such as Faraday/Kerr effects, linear birefringence, and magnetoelectric birefringence are evidence for broken symmetry states of matter. The recent discovery of a Kerr effect using near-IR light in the pseudogap phase of the cuprates can be regarded as a strong evidence for a spontaneous symmetry breaking and the existence of an anomalous long-range ordered state. In this work we present a high precision study of the polarimetry properties of the cuprates in the THz regime. While no Faraday effect was found in this frequency range to the limits of our experimental uncertainty (1.3 milli-radian or 0.07°), a small but significant polarization rotation was detected that derives from an anomalous linear dichroism. In $\text{YBa}_2\text{Cu}_3\text{O}_y$ the effect has a temperature onset that mirrors the pseudogap temperature T^* and is enhanced in magnitude in underdoped samples. In $x=1/8$ $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, the effect onsets above room temperature, but shows a dramatic enhancement near a temperature scale known to be associated with spin and charge ordered states. These features are consistent with a loss of both C_4 rotation and mirror symmetry in the electronic structure of the CuO_2 planes in the pseudogap state.

Superconductivity and magnetism in epitaxially grown Bi/Ni bilayers

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The coexistence of superconductivity and ferromagnetism has long been an interesting topic in condensed matter physics. Although neither Bi nor Ni bulk material shows superconductivity, the Bi/Ni bilayers are indeed superconducting and possible coexisting with ferromagnetism [1]. However many questions remain unanswered. With the MBE grown samples we have conducted systematically the transport and magnetic measurements. In this talk, I will present our results exhibiting some novel and unexpected behaviours of this system, which might be connected with the nontrivial topological properties of Bi thin films [2,3].

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Point-contact spectroscopy study of the pairing symmetry of candidate topological superconductors

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The recently proposed topological superconducting materials are predicted to exhibit p_x+ip_y pairing symmetry and host Majorana fermions on the surface. Here we investigate the pairing symmetry of candidate topological superconductors, including $\text{Cu}_x\text{Bi}_2\text{Se}_3$, $\text{Sn}_{1-x}\text{In}_x\text{Te}$, etc., via point-contact spectroscopy. The measurements are performed using both normal-metal gold tips and s-wave superconducting niobium tips. For samples with s-wave pairing, one would expect standard Andreev reflection in the gold tip case and supercurrent-like behavior in the niobium tip case. For $\text{Cu}_x\text{Bi}_2\text{Se}_3$, however, we observe robust zero-bias conductance peak (ZBCP) in the differential conductance spectra with gold point contact, while with niobium point contact we find the height of the peak exhibiting an unusual non-monotonic temperature dependence. We argue that both observations cannot be explained by Andreev reflection within the standard s-wave BTK model, but signifying unconventional superconductivity in this material. For $\text{Sn}_{1-x}\text{In}_x\text{Te}$ samples, we observe unexpectedly strong ZBCP in the differential conductance spectra with gold point contact, while with niobium point contact, the temperature dependence of ZBCP is monotonic as expected from conventional theory, leaving the nature of the superconductivity of $\text{Sn}_{1-x}\text{In}_x\text{Te}$ still an open question.

Key words: topological superconducting materials, point-contact spectroscopy, pairing symmetry, Andreev reflectionref

Evidences of polaron formation in high temperature superconducting copper oxides: phonon renormalization, isotope effects, multiband signatures, NMR and NQR anomalies

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High temperature superconducting copper oxides are frequently understood in terms of electronic correlation effects, spin fluctuation mechanisms, Hubbard and t-J models. However, lattice effects, electron-lattice coupling and polaronic effects play a fundamental role in the pairing mechanism, as evidenced from unconventional isotope effects, lattice anomalies on an average and local scale, substantial heterogeneities, phonon anomalies, NMR and NQR deviations from BCS theory, possible multiband effects. A consistent picture for understanding these features is obtained by considering strong electron-lattice interactions as major player in these complex materials, where polaron formation takes place and leads to important renormalizations of electronic and lattice degrees of freedom. Especially unconventional isotope effects arise in this scenario together with local lattice instabilities consistent with experimental data. The multiband properties appear as a consequence of substantial heterogeneity and lead to a mixed order parameter picture where s+d pairing is realized. Further important properties as phonon anomalies and those related to NMR and NQR data are discussed.

Resonant Soft X-ray Scattering Study of Charge Density Wave Correlations in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

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I will present a systematic study of the Charge-Density-Wave (CDW) correlations in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ (YBCO) over a wide range of doping ($0.4 < x < 0.93$). The CDW correlations are observed by means of Cu- L_3 edge resonant soft x-ray scattering in crystals with oxygen contents higher than 0.45 (corresponding to a hole concentration $p \approx 0.086$). The intensity, correlation lengths, and onset temperatures of the CDW increase smoothly with increasing doping, and get maximized around $p \approx 0.12$. All these quantities decrease again towards optimal doping. The incommensurability of the CDW wave-vector q_{CDW} increases linearly with doping, as recently reported for other cuprates families, but in sharp contrast with the doping dependence of the charge stripes observed in the 214 family. Moreover, in agreement with previous studies, an applied magnetic fields enhances the CDW signal, but only for doping levels above $p \approx 0.09$. On the contrary, at the lowest doping levels showing CDW, a static magnetic order develops and is enhanced by applied magnetic field. This is consistent with a picture where charge and spin incommensurate orders compete with each other and with superconductivity in the underdoped region of the phase diagram of YBCO.

The presented results are of paramount importance in the frame of a unifying picture for charge order in cuprates. However the differences between YBCO and other cuprates reported here might suggest the fact that, behind a very similar phenomenology, distinct, system dependent, microscopic origins can lead to charge modulations in doped CuO₂ planes.

Keywords: CDW, cuprates, Resonant Soft X-ray Scattering

CHAPTER VI

Poster Session

ARPES and core-level spectroscopies of the coexistence of ferromagnetism and superconductivity in Sr₂VFeAsO_{3- δ}

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The iron-based superconductor Sr₂VFeAsO_{3- δ} shows a relatively high superconducting transition temperature (T_c) of 37 K for $\delta = 0$ [1]. While the Fe 3d electrons are responsible for the superconductivity, Mott-insulator-like behavior has been proposed for the V 3d electrons [2]. When oxygen deficiencies of $\delta = 0.5$ are introduced, T_c decreases to 20 K and a weak ferromagnetism appears with a Curie temperature $T_C \sim 240$ K and a magnetic moment $\sim 0.1\mu_B/V$ [3]. Although this weak ferromagnetism has been associated with a canted magnetic moment of the V atom, the detailed mechanism of the ferromagnetism is still unclear. Also, the oxygen-deficiency induced change in the electronic structure has not been studied so far. In this study, we have performed measurements of angle-resolved photoemission spectroscopy (ARPES) and core-level spectroscopies on single crystals of Sr₂VFeAsO_{3- δ} ($\delta = 0, 0.5$). From V 2p X-ray photoemission and absorption (XPS and XAS, respectively), the valence state of V atom was suggested to be close to 3+ in both samples. Figure 1 shows the ARPES spectra around the Γ point measured at $T = 40$ K. Although the shift due to the electron doping from the oxygen deficiencies was not seen clearly, the spectral intensity of the band α was enhanced in the $\delta = 0.5$ sample.

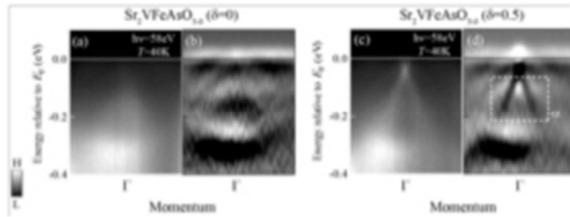


Fig. 1: ARPES spectra of $\text{Sr}_2\text{VFeAsO}_{3-\delta}$ around the Γ point (left) and its second derivative (right). (a), (b) $\delta=0$. (c), (d) $\delta=0.5$.

key words: iron-based superconductor, ferromagnetism, ARPES

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Electrostatically Induced Superconductivity under Pressure

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Unconventional superconductivity is among one of the most widely researched areas in condensed matter physics today and much progress is being made toward understanding this phenomena. Chemical doping generally provides the most common method for tuning into such a superconducting state yet can be difficult to control and also potentially introduces structural disorder complicating the underlying physics. [1, 2] Electric Double Layer devices provide a means to electrostatically dope materials with high electric fields allowing continuous tuning of the superconducting state as well as avoiding any structural issues. One such device is the Electric Double Layer Capacitor which can detect the onset of superconductivity through AC magnetisation measurements. [3] We make use of a similar device in an attempt to electrostatically dope and tune the superconductivity in the cuprate compound $\text{La}_{1.93}\text{Sr}_{0.07}\text{CuO}_4$ as well as investigating whether application of pressure improves its efficiency.

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Keywords: electrostatically, superconductivity, pressure

d+ip wave superconductivity in the AF state of layered cuprates

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We study the formation of the spin triplet component of the superconducting order parameter, which arises in the coexistence region of dx²+y² superconductivity (SC) and spin density wave

(SDW) within a mean-field treatment. For small electron doping the spin triplet component has p-wave symmetry yielding in total the d + ip superconducting gap. At larger doping the spin triplet component remains non-zero but changes symmetry towards d-wave wave gap resulting in higher harmonic contribution to the spin singlet d-wave gap. We further analyze the transverse and longitudinal spin excitation spectrum and the superfluid density of the system with special emphasis on the effect of the spin triplet component.

Keywords: spin density wave, unconventional superconductivity, competing phases

Superconductivity from repulsion in LiFeAs: novel s-wave symmetry and potential time-reversal symmetry breaking

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We analyze the structure of the pairing interaction and superconducting gap in LiFeAs by decomposing the pairing interaction for various k_z cuts into s- and d-wave components and by studying the leading superconducting instabilities. We use the ten orbital tight-binding model, derived from ab-initio LDA calculations with hopping parameters extracted from the fit to ARPES experiments. We find that the pairing interaction almost decouples between two subsets, one consists of the outer hole pocket and two electron pockets, which are quasi-2D and are made largely out of d_{xy} orbital, and the other consists of the two inner hole pockets, which are quasi-3D and are made mostly out of d_{xz} and d_{yz} orbitals. Furthermore, the bare inter-pocket and intra-pocket interactions within each subset are nearly equal. In this situation, small changes in the intra-pocket and inter-pocket interactions due to renormalizations by high-energy fermions give rise to a variety of different gap structures. We find four different configurations of the s-wave gap immediately below T_c . We discuss the phase diagram and experimental probes to determine the structure of the superconducting gap in LiFeAs. We argue that the state with opposite sign of the gaps on the two inner hole pockets has the best overlap with ARPES data. We also argue that at low T , the system may enter into a "mixed" s + is state and time-reversal symmetry is spontaneously broken.

Keywords: pnictides, multi-band superconductor, pairing symmetries, phase diagrams, time-reversal symmetry breaking

Fluctuations in pump-probe experiments

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The pump-probe scheme is the standard tool to get access to the time-domain response of out-of-equilibrium systems. One of the observables that can be probed as a function of the delay between the exciting laser pulse and the probe one is the reflectivity of the sample. The measurement of the reflectivity at each pump-probe delay occurs many times every second, since the pulsed laser sources usually work at high repetition rates.

However, out of all these measurements, only the average reflectivity at a given pump-probe delay is retained. The fluctuations of the outcomes of the measurements, i.e. their distribution, are usually discarded. I will present pump-probe measurements, performed on a bismuth crystal, of the time evolving fluctuations of the out-of-equilibrium reflectivity, showing how they carry additional information on the dynamics occurring in the sample.

Proximity effect of antiferromagnetism on superconductivity in the phase-separated ternary iron selenides $K_yFe_{2-x}Se_2$

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We examine superconductivity in the mesoscopically mixed antiferromagnetic (AF) and superconducting (SC) phases of ternary iron selenides $K_yFe_{2-x}Se_2$. It is shown that the interlayer hopping and AF order are key factors to determine T_c of the SC phase. In general, the hopping will produce deformed Fermi surfaces that tend to suppress superconductivity. However, contrary to the common expectation, we find that a larger AF order actually results in a larger SC order, which explains the observed relatively high T_c in these phases. Furthermore, our results indicate that by reducing the interlayer hopping appropriately, phase-separated $K_yFe_{2-x}Se_2$ may exhibit its intrinsic SC phase in the two-dimensional limit with a much higher T_c (~ 65 K) than what has been observed.

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Low energy effective Hamiltonian in iron based superconductors lacking inversion symmetry

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We investigate the effect of the lack of inversion symmetry, such as at the surface, on the low energy, effective Hamiltonian for electronic states near the Fermi level in iron based superconductors. We use the method of invariants to determine a small k expansion near the Γ and M points in the Brillouin zone for the two iron unit cell. Notably, we highlight differences between our results and those which use an inversion symmetric unit cell.

Keywords: FeSe, method of invariants, inversion breaking

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