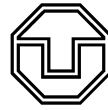


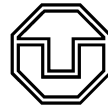
2nd WORKSHOP IMS2017

INTERMITTENT MAGNETISM AND SUPERCONDUCTIVITY

DRESDEN, GERMANY | SEPTEMBER 28-29, 2017







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1. PREFACE

Welcome to the second international workshop “Itinerant Magnetism and Superconductivity”. The aim of this workshop is to exchange and discuss recent advances and new ideas in the research on unconventional superconductors and complex correlated electron systems. It brings together leading experts as well as young researchers working in the field of iron-based superconductors, unconventional superconductivity in general, and related topological phases.

This workshop is organized by the Deutsche Forschungsgemeinschaft (DFG) research training group “Itinerant magnetism and superconductivity in intermetallic compounds” (GRK 1621). In this research training group, since 2011 more than 30 PhD students have been and will be doing research in an interdisciplinary initiative. They are guided and supported by more than 20 young as well as experienced researchers from chemistry and physics in a coordinated initiative to advance science in this exciting field.

We are grateful to all participants for sharing their recent results and we hope you will enjoy the workshop as well as your stay in Dresden.

Hans-Henning Klauß (TU Dresden)

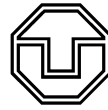
on behalf of the members of the GRK 1621

2. TIMETABLE

Time	Thursday, Sept 28
08:00-08:50	Registration
08:50-09:00	Welcome and Introduction
	S1: Dynamics and nematics in superconductors
09:00-09:35	1.1: Michael Sentef : Theory of ultrafast dynamics in superconductors
09:35-10:10	1.2: Ian R. Fisher : Anisotropic strain: an important means to probe and tune nematic phases
10:10-10:45	1.3: Nicolas Curro : NMR studies of nematic order and fluctuations in the iron pnictides
10:45-11:15	Coffee break
	S2: Unconventional superconductivity
11:15-11:50	2.1: Maria Navarro Gastiasoro : Disorder effects in correlated superconductors
11:50-12:25	2.2: Ni Ni : New additions to the Fe pnictide superconductors: recent progress in the 112 and 1144 superconducting families
12:25-14:00	Lunch break
	S3: Magnetism and superconductivity in iron-based superconductors
14:00-14:35	3.1: Markus Braden : Anisotropic resonance modes emerging in an antiferromagnetic superconductor
14:35-15:10	3.2: Jitae Park : Spin dynamics studies on heavily electron-doped iron-selenide superconductors
15:10-15:40	Coffee break
	S4: Thin films
15:40-16:15	4.1: Kazumasa Iida : Electric double layer transistor in NdFeAsO and grain boundary junctions of NdFeAs(O,F)
16:15-16:50	4.2: Jens Hänisch : High-field transport properties of Fe-based superconducting thin films
16:50-17:15	4.3: Stefan Richter : Superconducting properties of Ni doped BaFe ₂ As ₂ thin films
17:15-19:15	Poster session
19:30	Dinner



Time	Friday, Sept 29
	S5: Topological states of matter
09:00-09:35	5.1: Gabor Halász: Probing Majorana nodal structures in Kitaev spin liquids
09:35-10:10	5.2: Vadim Grinenko: Superconductivity with broken time reversal symmetry in $Ba_{1-x}K_xFe_2As_2$ single crystals
10:10-10:45	5.3: Ilya Eremin: Cooper-pairing with small Fermi energies in multiband superconductors: BCS-BEC crossover and time-reversal symmetry broken state
10:45-11:15	Coffee break
	S6: Time-reversal Symmetry Breaking
11:15-11:50	6.1: Egor Babaev: Properties of s+is superconductors: type-1.5 superconductivity, skyrmions and collective modes
11:50-12:25	6.2: Yuriy Yerin: Soliton states in a three-band superconductor with broken time-reversal symmetry
12:25-13:30	Lunch break
	S7: Photoemission, high pressure phases
13:30-14:05	7.1: Inna M. Vishik: ARPES studies on Hg1201
14:05-14:30	7.2: M. O. Ajeesh: Tuning competing ground states in $LuFe_4Ge_2$ using external pressure
14:30-14:55	7.3: Monika Güttler: Brillouin zone folding across the antiferromagnetic transition in $EuRh_2Si_2$
14:55-15:00	Concluding remarks



3. ABSTRACTS OF TALKS

3.1 Session 1: Dynamics and nematics in superconductors

3.1.1. Theory of ultrafast dynamics in superconductors

Michael Sentef

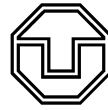
Max-Planck-Institut für Struktur und Dynamik der Materie, 22761 Hamburg, Germany

Understanding the collective motion of electrons in solids and their interplay with lattice vibrations is a central goal of condensed matter physics. Time-domain spectroscopies with tailored laser pulses offer novel ways to manipulate emergent ordering phenomena in superconductors or charge-density waves. Here I will show recent progress in the theoretical description of ultrafast dynamics in superconductors. I will discuss collective Higgs modes that can be excited in optically pumped electron-phonon superconductors [1]. Motivated by experiments that control electrons via resonant driving of the crystal lattice, I will then show how light-enhanced superconductivity plays out in the time domain [2]. Finally, I will show how lasers can control competing superconducting and charge-density wave states [3].

[1] A. F. Kemper et al., Phys. Rev. B 92, 224517 (2015).

[2] M. A. Sentef et al., Phys. Rev. B 93, 144506 (2016).

[3] M. A. Sentef et al., Phys. Rev. Lett. 118, 087002 (2017).

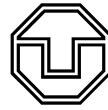


3.1.2 Anisotropic strain: an important means to probe and tune nematic phases

I. R. Fisher

Stanford University, Department of Applied Physics and Geballe Laboratory for Advanced Materials, CA 94305

Strongly anisotropic electronic states are observed for several families of strongly correlated quantum materials and high temperature superconductors. At least for Fe based superconductors, we now understand that the pervasive structural phase transition that is found for underdoped compositions of these materials is driven by electronic nematic order, raising the question of what role, if any, nematic fluctuations play in the superconducting pairing interaction. Since nematic order couples bilinearly to anisotropic strain with the same symmetry, it is clear that antisymmetric strain can play a special role in the investigation of such materials. In this talk I will outline recent advances in the study of electronic nematicity, first in terms of elastoresistance measurements (i.e. measurements that probe the change in resistivity due to induced strains of various symmetries), and second in using anisotropic strain as an effective tuning parameter for nematic order.



3.1.3 NMR studies of nematic order and fluctuations in the iron pnictides

Nicholas Curro

University of California, Physics Department, Davis, CA

Nuclear Magnetic Resonance of the As-75 offers unprecedented insight into the low energy spin and charge dynamics present in the iron pnictide superconductors. I will present data on both Co-doped and P-doped BaFe₂As₂ that uncovers some of the unusual physics associated with the nematic ordering present in this family of materials. The As-75 is sensitive to both the spin degrees of freedom via the hyperfine interaction, as well as the nematic degrees of freedom via the quadrupolar moment of the nucleus. By comparing As and P NMR, we can access the dynamical nematic susceptibility. Furthermore, by applying uniaxial strain in the paramagnetic phase, we are able to access the static nematic susceptibility.

3.2 Session 2: Unconventional superconductivity

3.2.1 Disorder effects in correlated superconductors

Maria Navarro Gastiasoro

School of Physics & Astronomy, Minneapolis, USA

We study the effects of disorder on unconventional superconductors in the presence of correlations, and explore a completely different disorder paradigm dominated by strong deviations from standard AG theory due to generation of local bound states and cooperative impurity behavior driven by Coulomb interactions. Specifically we explain under which circumstances magnetic disorder acts as a strong poison destroying high- T_c superconductivity at the sub-1% level, and when non-magnetic disorder, counter-intuitively, hardly affects the unconventional superconducting state while concomitantly inducing an inhomogeneous full-volume magnetic phase. Recent experimental studies of Fe-based superconductors have discovered that such unusual disorder behavior seem to be indeed present in those systems.



3.2.2 New additions to the Fe pnictide superconductors: recent progress in the 112 and 1144 superconducting families

Ni Ni

University of California, Department of Physics and Astronomy, Los Angeles

Both cuprates and Fe-based superconductors, the two known high T_c superconducting families, show rich emergent phenomena near the superconductivity (SC). To understand the mechanism of unconventional SC, it is crucial to unravel the nature of these emergent orders. Recently, two new Fe pnictide superconducting families are discovered. One is the 112 family whose global C_4 rotational symmetry is broken even at room temperature, the other is the 1144 family. As new additions to the Fe pnictide superconductors, they show unique properties. In this talk, I will discuss and review the current research progress in the study of both 112 and 1144 families.

3.3 Session 3: Magnetism and superconductivity in iron pnictides

3.3.1 Anisotropic resonance modes emerging in an antiferromagnetic superconductor

Markus Braden¹, Florian Waßer¹, Navid Qureshi¹, Paul Steffens², Chul-Ho Lee³, K. Kihou³, Yvan Sidis⁴, Sabine Wurmehl⁵ and B. Büchner⁵

¹II. Physikalisches Institut, Universität zu Köln, Germany; ²Inst. Laue Langevin, Grenoble, France; ³AIST, Tokyo, Japan; ⁴Laboratoire Léon Brillouin, Gif sur Yvette, France; ⁵IFW, Dresden, Germany.

There are two key features suggesting magnetically driven unconventional superconductivity in various systems: firstly the phase diagrams show the closeness or even coexistence of superconducting and magnetically ordered phases, and secondly magnetic spin-resonance modes appear at the onset of superconductivity. It appears thus most interesting to study the combination of these two features, the emergence of spin-resonance modes in an antiferromagnetic superconductor.

This problem can be well studied in underdoped BaFe₂As₂, for which the local coexistence of large moment antiferromagnetism and superconductivity is well established by local probes such as NMR and μ SR. Several unpolarized neutron scattering studies for Co doping of about 4.5% reveal a broad spin-resonance feature in the superconducting state but could not identify the nature of this signal. We have applied the polarization analysis in our neutron scattering experiments, which allows us to separate and identify the anisotropies of the magnetic excitations.

In the normal state of Co underdoped BaFe₂As₂ the antiferromagnetic order results in broad magnetic gaps opening in all three spin directions that are reminiscent of the magnetic response in the parent compound [1], where magnetic anisotropy arising from spin-orbit coupling results in sizeable magnetic gaps. In the superconducting state of the underdoped material two distinct anisotropic resonance excitations can be identified, but in contrast to numerous studies on optimum and over-doped BaFe₂As₂ [2,3] there is no isotropic resonance excitation [4], in particular there is no longitudinal contribution to the superconducting resonance. The two anisotropic resonance modes appearing within the antiferromagnetic phase are attributed to a selective superconducting state emerging in the band structure of the antiferromagnetic phase, in which longitudinal magnetic excitations are already gapped by the antiferromagnetic order with sizeable moment [4].

These results further document the importance of spin-orbit coupling for the low-energy magnetic properties of doped BaFe₂As₂ [5].

[1] N. Qureshi et al., Phys. Rev. B 86, 060410 (2012);

[2] P. Steffens et al., Phys. Rev. Lett. 110, 137001 (2013);

[3] N. Qureshi et al., Phys. Rev. B 90, 100502(R) (2014);

[4] F. Waßer et al., arXiv:1609.02027; [5] F. Waßer et al., Phys. Rev. B 91, 060505(R) (2015).

3.3.2

Spin dynamics study on heavily electron-doped iron-selenide superconductors

Jitae Park

Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM-II)
Technical University Munich, 85748 Garching, Germany

Heavily electron-doped iron-selenide (HEDIS) superconductors with a relatively high T_c , including monolayer FeSe thin film ($T_c > 50\text{K}$), alkali-metal intercalated 122-type FeSe ($T_c \simeq 32\text{K}$), and newly discovered phase-pure $\text{Li}_{0.8}\text{Fe}_{0.2}\text{OHFeSe}$ ($T_c \simeq 41\text{K}$), possess a peculiar electronic structure different from typical Fe-based superconductors: No hole-like Fermi surface at the center of Brillouin zone. Such feature immediately challenges the sign-reversed s-wave (s_{\pm}) pairing symmetry, which was originally proposed for Fe-based superconductors based on presence of both electron and hole Fermi pockets. The exact physical origin of a notably high transition temperature in the HEDIS without the hole Fermi pocket is not yet understood. Our recent inelastic neutron scattering studies on magnetic fluctuations in a series of sulfur-doped superconducting 122-FeSe and deuterated $\text{Li}_{0.8}\text{Fe}_{0.2}\text{ODFeSe}$ (11111) single crystals revealed the magnetic resonant mode in both systems, confirming that the superconducting gap function still contains sign-reversal structure. In the 122-FeSe, the magnetic resonant mode appears at $(\pi, 0.5\pi)$ wave vector and below 2 times of superconducting energy gap magnitude, but the resonant mode gradually smears out into the particle-hole continuum upon increase of sulfur-doping, indicating a possible change of the pairing channel. In 11111, nearly ring-shaped resonant excitations have been found at $(\pi, 0.625\pi)$ and at the energy of 21 meV below T_c , and high-energy spin excitations show the twisted dispersion across ~ 60 meV towards the (π, π) similar to those of hole-doped cuprates. In this talk, we will discuss physical implication on our experimental observations.

3.4 Session 4: Thin films

3.4.1 Electric double layer transistor in NdFeAsO and grain boundary junctions of NdFeAs(O,F)

Kazumasa Iida^{1,2}, Takuya Matsumoto¹, Taito Omura², Takahiro Urata^{1,2}, Takafumi Hatano^{1,2}, Hiroshi Ikuta^{1,2}

¹ Department of Materials Physics, Nagoya University, ² Department of Crystalline Materials Science, Nagoya University

To date most of the iron-based superconducting single crystals and thin films have been fabricated due to the great progress of fabrication process. We have also successfully grown high quality, epitaxial thin films of NdFeAs(O,F) on various substrates by molecular beam epitaxy (MBE)[1], which gives a lot of opportunities for applied and fundamental research [2-3]. In our fabrication a primary deposition at 800°C produced mother compound NdFeAsO. Subsequently, NdOF over-layer was deposited at the same temperature, from which fluorine was diffused into the NdFeAsO layer. Interestingly, NdFeAsO deposited on CaF₂(100) substrate showed an onset superconductivity without NdOF over-layer. Hall effect measurements revealed that the dominant carrier type was p-type. Hence hole doping into NdFeAsO/CaF₂ may enhance the superconducting transition temperature (T_c). For this purpose we prepared an electric double layer transistor in parent compound NdFeAsO in order to dope high-density charge carriers. Despite the hole injection by applying a negative gate, T_c of NdFeAsO/CaF₂ was not enhanced. Later we identified the origin of superconductivity arising from fluorine from CaF₂ substrate.

We also fabricated NdFeAs(O,F) on [100]-tilt MgO bicrystal substrates for evaluating inter-grain transparency across the grain boundary (GB). Unlike Co-doped BaFe₂As₂[4] and Fe(Se,Te)[5], the decay of inter-grain critical current density (J_c) is rather significant due probably to the erosion of GB by fluorine. In this talk, the aforementioned two topics will be discussed more detail.

The work was partially supported by the JSPS Grant-in-Aid for Scientific Research (B) Grant Number 16H04646.

[1] T. Kawaguchi *et al.*, *Appl. Phys. Express* **4**, 083102 (2011); T. Kawaguchi *et al.*, *Appl. Phys. Lett.* **97**, 042509 (2010); H. Uemura *et al.*, *Solid State Commun.* **152**, 735 (2012).

[2] K. Iida *et al.*, *Appl. Phys. Lett.* **105**, 172602 (2014).

[3] C. Tarantini *et al.*, *Sci. Rep.* **6**, 36047 (2016).

[4] S. Lee *et al.*, *Appl. Phys. Lett.* **95**, 212505 (2009); T. Katase *et al.*, *Nat. Commun.* **2**, 409 (2011).

[5] E. Sarnelli *et al.*, *Appl. Phys. Lett.* **104**, 162601 (2014); W. Si *et al.*, *ibid.* **106**, 032602 (2015).

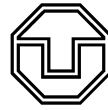
3.4.2 High-field transport properties of Fe-based superconducting thin films

Jens Hänisch,¹ Kazumasa Iida,² Fritz Kurth,³ Stefan Richter,³ Ruben Hühne,³ Vadim Grinenko,⁴ Bernhard Holzapfel,¹ Ludwig Schultz³

¹ Institute for Technical Physics, Karlsruhe Institute of Technology, ² Department of Crystalline Materials Science, Graduate School of Engineering, Nagoya University, ³ Institute for Metallic Materials, IFW Dresden, ⁴ Institute for Solid State Physics, TU Dresden

Fe-based superconductors show great potential for low-temperature high-field applications, such as magnet coil inserts, due to their large upper critical fields and irreversibility fields as well as to their low electronic anisotropy. Especially members of the 122 family, such as Co-, Ni, and P-substituted BaFe_2As_2 are interesting due to their low Ginzburg numbers and 3D behavior in the whole temperature range.

This talk will give an overview on transport and flux pinning properties of these compounds in magnetic fields up to 60 T. Comparisons to other Fe-based superconductors, such as Fe(Se,Te) and $\text{REFeAs}(\text{O},\text{F})$ (RE rare earth) as well as cuprate superconductors are drawn.



3.4.3 Superconducting properties of Ni doped BaFe₂As₂ thin films

S. Richter^{1, 2}, F. Kurth, K. Iida, V. Grinenko, S. Aswartham, K. Pervakov, C. Tarantini, J. Jaroszynski, A. Pukenas, J. Hänisch, S. Wurmehl, B. Büchner, W. Skrotzki, K. Nielsch, R. Hühne

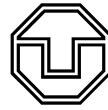
¹ Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, Germany

² Technische Universität Dresden, Germany

Iron based superconductors show appealing properties for future high field applications due to its small electronic anisotropy and high upper critical fields. At the same time, the interplay of superconductivity and magnetism in these multi-band systems is of fundamental interest to achieve a better understanding of high temperature superconductivity.

Furthermore, the variation of biaxial strain in thin films enables a deeper understanding in the connection between structure and functional properties.

In this talk we show results for Ba(Fe_{1-x}Ni_x)₂As₂ thin films, which have been epitaxially grown on substrates with different lattice constants. The observed maximum T_c of 21.4 K on CaF₂ is among the highest values reported for the Ni doped system. We will discuss the electronic phase diagram in comparison to single crystals and Co doped BaFe₂As₂ thin films. Additionally, the upper critical field and critical current density have been studied in static magnetic fields up to 35 T. These results were correlated afterwards with detailed microstructural investigations.



3.5 Session 5: Topological states of matter

3.5.1 Probing Majorana nodal structures in Kitaev spin liquids

Gabór Halász

University of California, Kavli Institute for Theoretical Physics, Santa Barbara

We propose that resonant inelastic X-ray scattering (RIXS) is an effective probe to detect the fractionalized excitations in two- and three-dimensional Kitaev spin liquids. While the non-spin-conserving RIXS responses are dominated by the gauge-flux excitations and reproduce the inelastic-neutron-scattering response, the spin-conserving (SC) RIXS response picks up the Majorana-fermion excitations and detects whether they are gapless at Dirac / Weyl points, nodal lines, or Fermi surfaces. As a signature of symmetry fractionalization, the SC RIXS response is suppressed around the Γ point for any Kitaev spin liquid on a bipartite lattice.

3.5.2 Superconductivity with broken time reversal symmetry in $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ single crystals

V. Grinenko^{1,2}, P. Materne¹, R. Sarkar¹, H. Luetkens³, K. Kihou⁴, C. H. Lee⁴, S. Akhmadaliev⁵, S. Aswartham², I. Morozov^{2,6}, D. V. Efremov², S.-L. Drechsler² and H.-H. Klauss¹

¹*Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany*

²*IFW Dresden, Helmholtzstrasse 20, 1069 Dresden, Germany*

³*Laboratory for Muon Spin Spectroscopy, PSI, CH-5232 Villigen PSI, Switzerland*

⁴*National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8568, Japan*

⁵*Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany*

⁶*Lomonosov Moscow State University, GSP-1, Leninskie Gory, Moscow, 119991, RF*

Over the past years a lot of theoretical and experimental effort has been made to find states with broken time-reversal symmetry (BTRS) in multiband superconductors. In particular, it was proposed that in the $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ system either an $s + is$ or an $s + id$ BTRS state may exist at high doping levels in a narrow region of the phase diagram. Here we report the observation of an enhanced zero-field muon spin-relaxation rate in the superconducting state below temperature T^* for a high quality crystalline sample with several K doping levels in the range $0.8 < x < 0.7$. [1] T^* is strongly doping dependent and is, usually, lower than the superconducting transition temperature T_c . Our observations are qualitatively consistent with theoretical predictions for BTRS state caused by frustrated interband pairing interactions. The symmetry of the order parameter in the BTRS state is discussed.

1. V. Grinenko, P. Materne, R. Sarkar, H. Luetkens, K. Kihou, C. H. Lee, S. Akhmadaliev, D. V. Efremov, S.-L. Drechsler, H.-H. Klauss, Phys. Rev. B 95, 214511 (2017).

3.5.3 Cooper-pairing with small Fermi energies in multiband superconductors: BCS-BEC crossover and time-reversal symmetry broken state

Ilya Eremin

Ruhr-Universität Bochum, Germany

In my talk I will consider the interplay between superconductivity and formation of bound pairs of fermions in multi-band 2D fermionic systems (BCS-BEC crossover). In two spatial dimensions a bound state develops already at weak coupling, and BCS-BEC crossover can be analyzed already at weak coupling, when calculations are fully under control. We found that the behavior of the compensated metal with one electron and one hole bands is different in several aspects from that in the one-band model. There is again a crossover from BCS-like behavior at $E_F \gg E_0$ (E_0 being the bound state energy formation in a vacuum) to BEC-like behavior at $E_F \ll E_0$ with $T_{ins} > T_c$. However, in distinction to the one-band case, the actual T_c , below which long-range superconducting order develops, remains finite and of order T_{ins} even when $E_F = 0$ on both bands. The reason for a finite T_c is that the filled hole band acts as a reservoir of fermions. The pairing reconstructs fermionic dispersion and transforms some spectral weight into the newly created hole band below the original electron band and electron band above the original hole band. A finite density of fermions in these two bands gives rise to a finite T_c even when the bare Fermi level is exactly at the bottom of the electron band and at the top of the hole band. I also analyze the formation of the $s+i$ state in a four-band model across the Lifshitz transition including BCS-BEC crossover effects on the shallow bands.

Similar to the BCS case, we find that with hole doping the phase difference between superconducting order parameters of the hole bands change from 0 to π through an intermediate $s+i$ state, breaking time-reversal symmetry (TRS).

3.6 Session 6: Time-reversal Symmetry Breaking

3.6.1 Properties of s+is superconductors: type-1.5 superconductivity, skyrmions and collective modes

Egor Babaev

KTH Royal Institute of Technology, Department of Theoretical Physics, Stockholm, Sweden

Breakdown of additional Z_2 symmetry in s+is superconductors results in a number of interesting properties, that will be overviewed in this talk. The properties of that superconducting state include:

- (i) Generic breakdown of type-1/type-2 dichotomy of superconducting state and appearance of a state where some coherence lengths are larger and some smaller than the magnetic field penetration length (termed type-1.5 state)
- (ii) Appearance of metastable Skyrmion excitations
- (iii) Change of collective modes and appearance of a mixed phase-density modes, instead of "phase-only" Leggett's mode
- (iv) Unconventional thermoelectric and flux flow properties

- [1] Phys. Rev. B 84, 134518 (2011).
- [2] Phys. Rev. Lett. 112, 017003 (2014).
- [3] Phys. Rev. Lett. 107, 197001 (2011).
- [4] Phys. Rev. B 87, 014507 (2013).
- [5] Phys. Rev. B 92, 174510 (2015).
- [6] Phys. Rev. Lett. 116, 097002 (2016).
- [7] Phys. Rev. B 88, 220504 (2013).
- [8] Phys. Rev. B 88, 220511 (2013).
- [9] Phys. Rev. B 89, 104509 (2014).
- [10] Phys. Rev. B 91, 140504 (2015).

3.6.2 Soliton states in a three-band superconductor with broken time-reversal symmetry

Y. Yerin^{1,2}

¹The Institute for Physics of Microstructures, Nizhny Novgorod, Russia ²B.Verkin Institute for Low Temperature Physics and Engineering
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Owing to the emergence of additional degrees of freedom of the order parameter, the nomenclature of topological objects in multiband superconductors is much richer than that in conventional single-band superconductors. Ginzburg-Landau theory describing multi-band superconductivity in bulk samples admit topologically stable solutions that can be interpreted as vortices carrying fractional magnetic flux. In the presence of Josephson-type interband coupling, multi-band superconductors generate static solitons of the sine-Gordon type [1,2 and references therein].

Solitons of the interband phase difference can exist by themselves in doubly-connected mesoscopic samples, when the formation of any magnetic vortices in the volume of the superconductor is prohibited energetically. Moreover, soliton states in this case can be induced by an externally applied magnetic field, which makes them a convenient object of the investigation.

Based on the Ginzburg-Landau phenomenological approach, we investigate soliton states in a three-band superconductor with broken time-reversal symmetry (BTRS). In comparison with other similar theoretical studies [1,2 and references therein] we consider the creation and characteristics of these solitons induced by external magnetic field for mesoscopic doubly-connected geometry (thin-walled cylinder) of a three-band superconducting system, which corresponds to the real experimental situation.

We demonstrate that due to the degeneration of energy minima of a BTRS three-band superconductor there are different types of solitons. Calculations of the Gibbs free energy of the system show that soliton states in a three-band superconductor with BTRS are thermodynamically metastable and cannot be the ground state for such geometry (fig. 1).

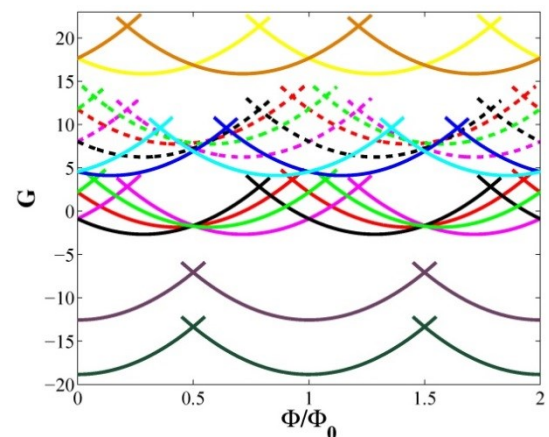


Fig. 1. Gibbs free energy of BTRS ground state (dark green), non-BTRS state (dark purple) and different topological states (N_1, n_2, n_3) for typical ratios of the effective masses $k_2 = 4$, $k_3 = 2$. Here red (solid and dashed) lines denote topological state with $(N_1, 1, 0)$, magenta (solid and dashed) – $(N_1, 0, 1)$, blue – $(N_1, 1, 1)$, yellow – $(N_1, -1, 1)$, brown – $(N_1, 1, -1)$, cyan – $(N_1, -1, -1)$, black (solid and dashed) – $(N_1, 0, -1)$ and green (solid and dashed) – $(N_1, -1, 0)$.

References

- 1) Shi-Zeng Lin, J. Phys.: Condens. Matter 26, 493202 (2014).
- 2) Y. Tanaka, Supercond. Sci. Technol. 28, 034002 (2015).

3.7 Session 7: Photoemission, high pressure phases

3.7.1 ARPES studies of Hg1201

Inna M Vishik

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HgBa₂CuO_{4+δ} (Hg1201) has been shown to be a model cuprate for scattering, optical, and transport experiments, but angle-resolved photoemission spectroscopy (ARPES) data are scarce owing to the absence of a charge-neutral cleavage plane. I will report on progress in achieving the experimental conditions where quantifiable ARPES spectra can be obtained. Studies of fermiology, superconductivity, and mode coupling will be discussed.

3.7.2 Tuning competing ground states in LuFe_4Ge_2 using external pressure

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Tuning of competing ground-state properties using external pressure has attracted much attention in current condensed matter research. This is due to the fact that, exotic phenomena and unconventional phases occur at regions of competing energy scales, especially in systems with magnetic frustration. Here, we investigate LuFe_4Ge_2 under external pressure in order to better understand the interplay between competing ground states. LuFe_4Ge_2 is a frustrated, itinerant magnetic system with antiferromagnetic (AFM) ordering accompanied by a structural transition at 36 K. The pressure dependence of the magneto-elastic transition in LuFe_4Ge_2 has been investigated using electrical transport, ac magnetic susceptibility, X-ray diffraction, Mössbauer, and muon-spin resonance (μSR) measurements under external pressure. External pressure suppresses the first-order magnetic transition (AFM1) at around 1.8 GPa, while the structural transition is largely unaffected by pressure. A new magnetic phase at higher pressures is confirmed by Mössbauer and μSR experiments. μSR data reveal that the full sample volume in the pressure-induced phase undergo long-range magnetic order. Mössbauer investigations at 2.9 GPa and in magnetic field indicate that the high pressure phase is also antiferromagnetically ordered (AFM2). In addition, different hyperfine magnetic fields obtained from Mössbauer data in the AFM1 and in the AFM2 region point at a different size of the ordered moment and/or a different magnetic structure in the two regions. Further studies to understand the pressure-induced phase and the interplay between magnetic and structural phase transitions are under way.

3.7.3 Brillouin zone folding across the antiferromagnetic transition in EuRh_2Si_2

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We studied the divalent Eu-based antiferromagnet EuRh_2Si_2 by means of high-resolution UV ARPES and soft X-ray ARPES. We found clear signatures of Brillouin zone and band folding across the antiferromagnetic transition at $T_N = 24.5$ K [1, 2] in the soft X-ray ($h\nu = 555 - 730$ eV) spectra. These findings are complemented and fortified by high-resolution Fermi surface maps ($h\nu = 45$ eV). The obtained Fermi surface topology in the AFM phase shows characteristic splittings, which can be attributed with the help of detailed bandstructure calculations to the folding of the two main Fermi surface sheets, the so-called *donut* and the *jungle-gym*. These sheets hybridize mutually upon their folding resulting in a non-trivial reconstruction of the Fermi surface across the AFM transition. Slab calculations show, that additional splittings in the ARPES Fermi surface arise from numerous spin-split surface resonances, which appear only in the vicinity of the broken symmetry of the surface and the top-most ferromagnetic Eu layer, similar to the previously studied Shockley surface states in EuRh_2Si_2 and GdRh_2Si_2 [3, 4].

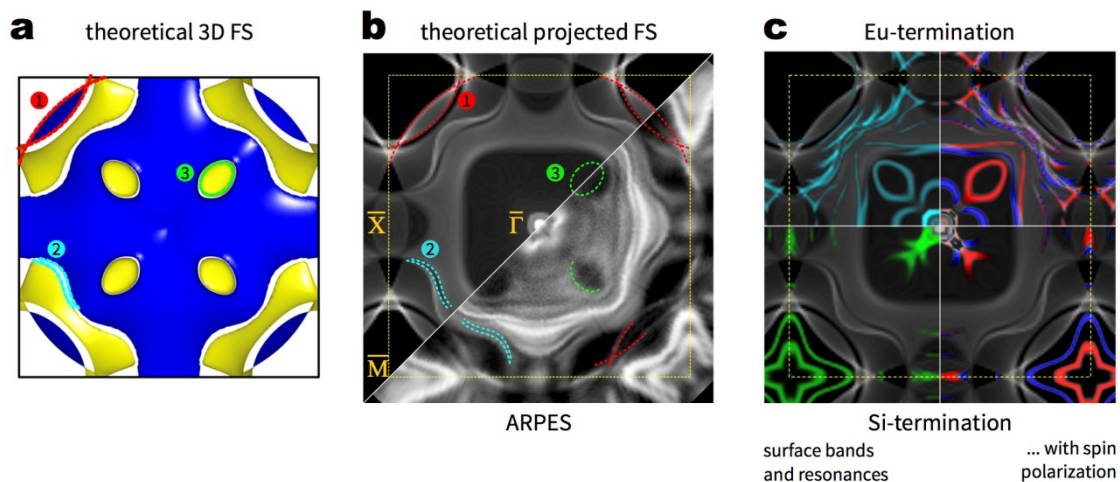


Fig. 1. (a) Calculated 3D Fermi surface (FS) in the AFM phase viewed along k_z . (b) Calculated projected FS compared to the FS obtained by ARPES with $h\nu = 45$ eV (corresponding to a Brillouin zone cut through Γ and nearby projected bands). (c) Combined bulk and slab calculations. Surface-related bands from Eu-termination (Si-termination) are shown in cyan (green). The spin polarization of the respective surface bands and resonances is indicated in red and blue.

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4. ABSTRACTS OF POSTERS

4.1 How ubiquitous are Bogoliubov Fermi surfaces for multiband superconductors?

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In general, it has been observed that in the absence of disorder or external magnetic field, the superconducting gaps are either nodeless or have point or line nodes. But it has been recently shown that nodal centro-symmetric multiband superconductors which spontaneously breaks time reversal symmetry (TRSB), generically have two-dimensional Fermi surfaces of Bogoliubov quasiparticles (“inflated” point or line nodes)[1-2]. These Fermi surfaces are Z_2 protected and are robust against any perturbation which is CP invariant. Our project concerns to address the question how common the Bogoliubov Fermi surfaces are and what controls their stability and also what will be the experimental signatures of these Bogoliubov Fermi surfaces. Our interest is to consider the pairing of $j=3/2$ fermion states, which is qualitatively different from the conventional pairing of $j=1/2$ states [3].

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4.2 Ferromagnetic order in a new 1144 iron-based superconductor investigated with NMR

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The recent discovery of two new iron-based superconductors - the so-called 1144 systems - enriches the list of ferromagnetic superconductors. These compounds crystallize in a structure similar to 122 systems. Their unique feature is that adjacent interlayers contain different atoms. Insertion of nonmagnetic atoms reproduce the main features of corresponding 122 materials, typically with higher superconducting T_c . However, the case of magnetic atoms opens possibilities for ferromagnetic (FM) order. It is well known that EuFe_2As_2 exhibits antiferromagnetic (AFM) order, with FM in-plane and AFM out-of-plane correlations. By substituting every second Eu layer with a nonmagnetic (Rb/Cs) layer, bulk ferromagnetism is achieved. We present characterization data of (Rb/Cs) EuFe_2As_2 powder samples as well as NMR spectroscopy and spin-lattice relaxation data. We find that magnetic field applied in NMR experiments enhances FM critical temperature to ~ 80 K which is much higher than the almost unaffected superconducting T_c .

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4.3 Pressure- induced metallization and Superconductivity in PdSe₂

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Transition Metal Dichalcogenides (TMDs) have been attracting an increasing attention among scientific community over the past few decades due to their intriguing physical properties and potential applications in electronics and optoelectronics. [1] The prosperity of (TMDs) MX₂ originates from their unique layered structural in which each layer is formed of a transition metal atom (M) sandwiched between two chalcogen (X: Se or S) via strong covalent bond. The layers are weakly stacked together through Van der Waals interactions leading to wide range of possible structural variations and electronic novel properties. Owing to these unique properties, external applied pressure would be a useful tool to tune such systems and in many cases inducing novel states of matter such as insulator-to-metal transition, CDW or superconductivity. [2,3] External applied pressure has proved to be clean, powerful technique that can tune compounds by altering the lattice parameters, and in turn changing the structural and electronic properties.

PdSe₂ can be considered as a prototypical example of TMDC due to their novel structure and electronic properties. PdSe₂ crystalizes at ambient pressure in an orthorhombic PdS₂-type layered crystal structure, space group Pbc_a and shows a semiconducting behavior with a sizeable indirect bandgap of ~ 0.25 eV. At high pressure, PdSe₂, however, crystalizes in the pyrite- type structure. [4] Tuning structure across the boundaries of quasi-2D and 3D system would be of interest to reveal the underlying physics and search for novel states of matter. Here, we present electrical transport measurement under pressure accompanied by Raman Spectroscopy. We also report an electronic driven insulator-to-metal transition without a structural phase transition. Applying further pressure drives the system into a dome-shaped pressure-induced superconductivity with maximum T_c of 13.1 K. Ab initio band structure calculations agrees with the experimental findings and even more interestingly indicate Dirac and nodal line fermions in the vicinity of Fermi energy.

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4.4 Muon Spin Relaxation studies of Sr_2RuO_4 under uniaxial pressure

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For two decades Sr_2RuO_4 has been discussed as a spin triplet p-wave superconductor, with a chiral order parameter of the form $p_x \pm ip_y$. This order parameter has not been proved yet, however one key piece of evidence is the observation of an enhanced zero-field muon spin relaxation rate in the superconducting state [1], which implies that the order parameter breaks time-reversal symmetry (TRS). Nevertheless, the absence of any measurable spontaneous magnetization in scanning SQUID studies raises questions about this interpretation [2]. T_c of Sr_2RuO_4 has been shown experimentally to be very sensitive to uniaxial pressure [3,4], so the changes in the muon spin relaxation rate with uniaxial pressure could provide further information both on the origin of the enhanced muon relaxation rate, and the superconductivity of Sr_2RuO_4 . Therefore, we have developed a uniaxial pressure cell for μSR . This cell is based on piezoelectric actuators, allowing continuous in situ tuning of the applied pressure. Here, we present results from our first set of measurements, in which we found that the low-temperature magnetic penetration depth has an unexpectedly sharp dependence on uniaxial pressure. We anticipate many further applications for this apparatus.

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4.5

Temperature vs pressure phase diagram of $\text{FeSe}_{1-x}\text{S}_x$ investigated using μSR

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Application of hydrostatic pressure to the iron based superconductor FeSe suppresses the nematic order and leads to the appearance of static magnetic order for pressures above 0.8 GPa [1]. At the same time, the superconducting T_c increases from 8 K at ambient pressure up to 37 K at approx. 7 GPa [2]. A recent study using high-pressure resistivity measurements suggests that isovalent S substitution for Se up to 17% leads to a faster suppression of the nematic phase while shifting the magnetic dome to higher pressures, which would lead to a complete separation of the two phases as a function of pressure [3]. Here, using muon spin rotation (μSR), we show however that static magnetism is already present at much lower pressures than previously thought in our slightly inhomogeneous sample with x ranging between 7% and 12%, although not with a full volume. In fact, the magnetism seems to develop already at slightly lower pressures than for pure FeSe. While the relatively large spread of S content in our sample makes quantitative estimation of the ordered moment size difficult, our data clearly indicate an increasing moment with increasing pressure, as it has been observed for FeSe, too. This study shows the usefulness of local probe magnetic measurements as a complementary technique.

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4.6 The Five-Orbital Hubbard Model - Tetragonal Magnetic Order and Superconductivity in Iron Pnictides

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Multiband and multiorbital physics is crucial for the understanding of superconductivity and magnetism in iron pnictides. We employ realistic multiorbital models to study the coexistence and competition of spin-density-wave (SDW) order and superconductivity and the newly discovered tetragonal magnetic phase in the 122-compounds $\text{Ba}_{1-x}\text{Na}_x\text{Fe}_2\text{As}_2$ [1] and $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ [2].

Avci et al. [1] report the observation of an additional fourfold-symmetric phase in $\text{Ba}_{1-x}\text{Na}_x\text{Fe}_2\text{As}_2$ by neutron powder diffraction. The new phase is close to the suppression of the SDW order. This discovery hints at a possible scenario: Magnetic interactions produce a spin-nematic phase, which induces orbital ordering of the iron 3d electrons.

Comparison with our previous work [3] will allow us to elucidate the role played by orbital effects. Hund's rule coupling is also crucial and will be included. We will also compare to other multiorbital systems.

We use a restricted Hartree-Fock method for studying multiorbital models with a large number of mean-field parameters. Handling that kind of systems can be challenging and numerically expensive. We enhance the usual tetrahedron method [4] by an adaptive refining algorithm to increase performance and work on a further development for finite temperature.

Furthermore, the question of how to calculate the proper set of mean-field parameters arose during our studies. Alongside with this project we investigate the use of minimization of the grand canonical ensemble to find mixed phases [5] and compare performance with the common iterative solution of the self-consistency equations.

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4.7 Spatial modulation of the superconducting order parameter: A microscopic study of the FFLO state in an all-organic superconductor

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The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state was theoretically predicted in 1964.^[1,2] It may be realized in materials when the orbital critical field exceeds the Pauli paramagnetic limit, and the mean free path is much larger than the coherence length. A hallmark of this state is the spatial modulation of the superconducting order parameter, caused by a strong population imbalance of a multi-component Fermi liquid. So far, experimental signatures of this exotic superconducting state were found in only very few materials.^[3,4]

Recently, microscopic evidence for spatially modulated superconductivity was found by nuclear magnetic resonance (NMR) spectroscopy.^[5,6] We report on our latest results of a comprehensive NMR study of the all-organic superconductor β'' -(ET)₂SF₅CH₂CF₂SO₃, with a focus on the phase diagram at magnetic fields exceeding the Pauli paramagnetic limit as determined from thermodynamic measurements. The spatial modulation of the spin susceptibility, anisotropy of the FFLO phase, as well as an enhancement of the nuclear spin-lattice relaxation rate, discussed as a signature of Andreev bound states, are addressed.^[7]

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4.8 Synthesis, structure and magnetic properties of new layered ternary compound in the Fe-As-Te system

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Being structurally similar to a number of already known layered mixed *d*-metal – *p*-element tellurides [1, 2], $\text{Fe}_{3+x}\text{AsTe}_2$ ($-0.4 < x < 0.3$) was assumed to have anisotropic electric conductivity and a low-dimensional magnetism with a T_C near room temperature [1, 3, 4]. The crystal structure of $\text{Fe}_{3+x}\text{AsTe}_2$ can be considered as a derivative of the NiAs type. It contains two different of Fe positions: fully occupied Fe(1) in trigonal bipyramidal voids and mixed, partially occupied Fe(2)/As in octahedral voids. The non-stoichiometry of this compounds arising from the partial occupancy of the Fe(2) site leads to slightly different structural patterns and composition-dependent properties of different samples [5].

$\text{Fe}_{3+x}\text{AsTe}_2$ was obtained by high-temperature ceramic technique from binary precursors, like FeTe_2 and Fe_2As . Single crystals of appropriate size and quality for structure solution and transport properties studies were usually grown by a three step recrystallization process starting from pre-synthesized powder.

The crystal structures in the composition range $\text{Fe}_{3+x}\text{AsTe}_2$ with $-0.4 < x < 0.3$ can be described as commensurately (3+1)-dimensional modulated in the monoclinic superspace group $P2_1/m(\alpha\beta 0)00$ describing the partial occupation of the Fe(2) positions in the *ab* plane. The modulation wave vector for a crystal of the composition Fe_3AsTe_2 is $q = (-1/3, -1/3, 0)$. The superspace approach was used to find a unified and consistent way to account for the slightly different compositions and to minimize the number of refineable parameters and, hence, possible correlations in the refinement.

Magnetization studies reveal ferromagnetic ordering with $T_C = 120$ K and a strong magnetocrystalline anisotropy along c^* . The low saturated moments of $\mu_s = 0.2 \mu_B/\text{Fe}$ at $T = 2$ K can be attributed to an increased dilution of the magnetic exchange between Fe(2) sites due to strong structural disorder. This feature turned out to be the key issue influencing the properties.

Magnetic susceptibility and Moessbauer spectroscopy studies evidence a complex magnetic structure consisting of at least two Fe sublattices and two ordered states with dominant ferromagnetic order of Fe(2) atoms above 25 K and dominating antiferromagnetic order of Fe(1) atoms below. Neutron scatterings are planned to uncover the magnetic structures.

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4.9 Cryo-EBSD on a BaFe₂As₂ single crystals and thin films

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Among iron-based high-temperature superconductors, BaFe₂As₂ is one of the most studied compounds in recent years [1]. The superconductivity can be induced either by carrier doping, chemical pressure, external pressure or epitaxial strain. In case of non-doped bulk BaFe₂As₂ material, there is a tetragonal-to-orthorhombic structural and magnetic phase transition below $T_c \approx 140$ K. The orthorhombic structure leads to the formation of twin lamellae. The results of previously published polarized light microscopy and transmission electron microscopy studies are inconsistent in observed lamella size [2, 3]. A scanning electron microscope with a cryogenic sample holder was combined with an electron backscatter diffraction technique to achieve high spatial resolution (≤ 100 nm) and to avoid any elaborated sample preparation prior to the analysis. The talk will present results of Cryo-EBSD on BaFe₂As₂ single crystals and epitaxial BaFe₂As₂ thin films.

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4.10 Magnetic properties and electronic correlations in BaTM_2As_2 (TM = Cr, Mn, Fe, Co, Ni, Cu)

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In order to better understand the multi-orbital nature of Fe-based superconductors in combination with strong electronic correlations in this class of materials, we report on a systematic investigation of the magnetic and thermodynamic properties of the isostructural series BaTM_2As_2 (TM=Cr, Mn, Fe, Co, Ni, Cu). Magnetization and specific heat measurements were performed on single crystalline samples to investigate the changes in the electronic and magnetic character and the degree of electronic correlation, varying the average occupancy of the 3d shell as a control parameter within the series. The results show that upon changing the occupation of the 3d orbitals, the electronic and magnetic character changes dramatically, which suggests a very complex interaction between on-site Coulomb repulsion, Hund's coupling and other competing effects. In particular the magnetic ground state shows a gradual change within the series, while the electronic correlation seems to be in accordance with what has already been suggested by theoretical as well as experimental contributions. [1-3] This work has been supported by Graduiertenkolleg GRK 1621.

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