# Book of Abstracts

# XVI National Conference on Superconductivity

October 7-12, 2013
Zakopane

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National Science Centre



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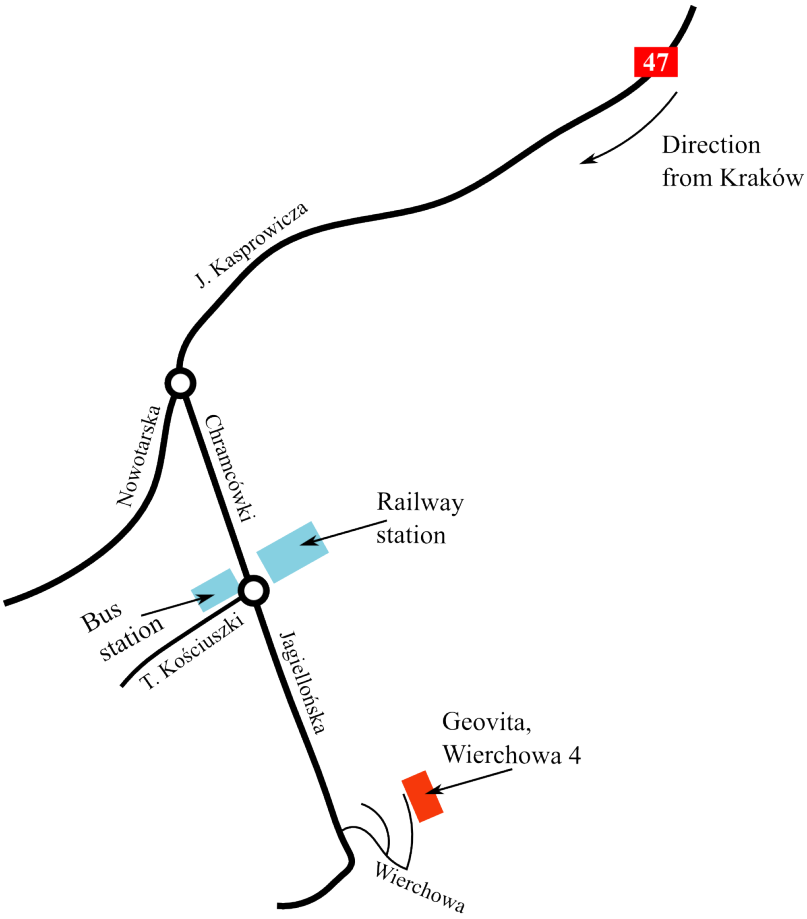
# How to get there




**By car:** Approaching Kraków via motorway A4 from the West just after pay toll (the A4 section from Katowice to Kraków is paid $2 \times 9$ PLN) keep to the right and take the first exit (direction: Kraków południe, Rzeszów). After 15 km leave the motorway by taking the exit to Chyżne (road number 7). Drive along road nr 7 for 56 km and then continue straight into road 47 (direction: Nowy Targ, Zakopane). After 40 km you arrive at the first roundabout visible in the picture above. Take the second exit into Chramcówki street and continue straight for 1,5 km. Then turn left into Wierchowa. After a short uphill drive you are right at Geovita!

**By plane:** After arriving in the Kraków-Balice airport there are three options to get to the city center: (i) take bus nr 292: you need the ticket for agglomeration (price 4 PLN); the bus leaves every 20 minutes; (ii) take the train (faster, but more expensive, around 20 PLN); (iii) take a taxi (should cost about 80 PLN). It is the best to go next to the Regional Bus Station in Bosacka 18. Both the 292 bus and train get very close to it. For 292 bus the stop name is "Dworzec Główny Wschód" and it takes 36 minutes for the bus to get there. The train stops on the train main station from which there are signs directing to the regional bus station "Regionalny Dworzec Autobusowy".

**By bus:** The Regional Bus Station is in Bosacka 18. From there are a few buses leaving to Zakopane every hour. The ticket price is around 20-30 PLN and the bus ride takes 2-2:30 hours. In Zakopane, the buses stop in Kościuszki street as indicated in the picture above.

**By train:** It is better not to go by train from Kraków, as the connection takes about 4 hours (twice the time needed by bus).

The persons who want to take the conference bus and who arrive and leave the Airport before 2 p.m. can take a taxi directly to the Institute of Physics of the Jagiellonian University, 4 Reymonta st., 30-059 Kraków.

Those arriving well before that time can take the 292 bus to "AGH" bus stop (the ride takes about 30 minutes), which is about 400 m from the Institute of Physics.

# XVI National Conference on Superconductivtity and Strongly Correlated Systems
# Zakopane 07/10 - 12/10/2013

## Conference Program

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| **$20^{00}$- $22^{00}$** | **Inaugural session:**<br><br>**Introduction by the representatives from the AGH University of Science and Technology, Prorector Zbigniew Kąkol, and from the Jagiellonian University, Dean Andrzej Warczak, about our Universities**<br><br>**Special lecture: Bogdan Sulikowski: Five-fold symmetry in science and art** |

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# Oral Presentations

# Strongly interacting Fermions and high $T_c$ superconductivity in the cuprates

Dirk van der Marel

*Département de Physique de la Matière Condensée, Université de Genève, Quai Ernest-Ansermet 24, 1201 Genève, Switzerland*

Cuprate high-$T_c$ superconductors exhibit enigmatic behavior in the nonsuperconducting state. On the overdoped side Fermi-liquid like characteristics are observed. For carrier concentrations near "optimal doping" (with respect to the highest $T_c$) the transport and spectroscopic properties are unlike those of a Landau–Fermi liquid. On the Mott-insulating side of the optimal carrier concentration, which corresponds to underdoping, a pseudogap removes quasi-particle spectral weight from parts of the Fermi surface and causes a breakup of the Fermi surface into disconnected nodal and antinodal sectors. Several anomalous behaviours are observed experimentally. Within the context of optical spectroscopy this is revealed by a temperature dependence of the free carrier spectral weight opposite to standard BCS behaviour.

Surprisingly, our recent optical experiments on very pure single crystals reveal that the quasi-particle relaxation rate $1/\tau(\omega, T)$ collapses on a universal function proportional to $(\hbar\omega)^2 + (p\pi k_B T)^2$, thus providing a piece of evidence in favor of a Fermi liquid-like scenario of the pseudogap phase of the cuprates. On the microscopic level, Fermi-liquid-like quasiparticle relaxation is the consequence of inelastic processes by which an electron decays under excitation of electron-hole pairs. Since the excitation spectrum of interacting electron-hole pairs corresponds to the susceptibility, $\chi"(\omega)$, aforementioned relaxation can be expressed by the electron-boson coupling function $I^2\chi"(\omega)$, added to the electron-phonon coupling, and coupling to other collective modes.

This function is loosely indicated as "glue spectrum", $\Pi(\omega)$. The latter can be downfolded from experimental optical spectra, and turns out to reveal a robust peak around 55 meV in addition to a broad continuum up to 0.5 eV. We observe a intriguing correlation between the experimental glue spectra and $T_c$ as a function of doping.

S. I. Mirzaei et al., PNAS 110, 5774-5778 (2013).
C. Berthod et al, PRB 87, 115109 (2013).
S. Dal Conte et al, Science 335, 1600-1603 (2012).
M. Guarise et al., PRL 105, 157006 (2010).
E. van Heumen et al, PRB 79, 184512 (2009).
F. Carbone et al, PRB 74, 064510 (2006).
D. van der Marel et al, Nature 425, 271-274 (2003).
H. J. A. Molegraaf et al, Science 295, 2239-2241 (2002).

## Unusual eletronic properties of iron arsenic high temperature superconductors

A. Kaminski[1], R. S. Dhaka[1], C. Liu[1], P. C. Canfield[1], and S. Bud'ko[1]

[1] *Ames Laboratory and Dept. of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA*

Many of the unconventional superconductors have complex phase diagrams, where the superconducting phase is often adjacent, or partially overlaps with an ordered state. Two best examples are cuprates and pnictides high temperature superconductors, where superconductivity partially coexists with pseudogap and antiferromagnetic state respectively.

The recently discovered iron arsenic high temperature superconductors exhibit particularly rich and interesting phase diagrams. We found that dramatic changes in the Fermi surface (Lifshitz transitions) coincide with the key transition lines in the phae diagram. We also found that the bands shift in energy with temperature, which likely assists the thermal fluctuations in destroying the AFM order. Recently, progress in sample preparation techniques allowed stabilize Collapsed Tetragonal phase (normally existing only under pressure) in ambient condition. This created opportunity to study its electronic properties and find clues why this phase does not support superconductivity.

## Quantum critical superconductivity in $Ce_2PdIn_8$

Dariusz Kaczorowski

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$Ce_2PdIn_8$ is an ambient-pressure heavy-fermion superconductor that in many aspects closely resembles the structurally related compound $CeCoIn_5$. This striking similarity stimulates comprehensive experimental investigations of this novel material with a variety of bulk and local probe techniques.

In my talk, I shall briefly review the experimental results hitherto obtained for single-crystalline and polycrystalline samples of $Ce_2PdIn_8$ with the main emphasis put on: (i) *non-Fermi liquid features* in the normal state, evidenced in electrical transport, heat capacity, $^{115}$In nuclear quadrupole resonance (NQR), and inelastic neutron scattering (INS) measurements; (ii) the occurrence of *magnetic-field-induced quantum critical point* near the upper critical field, seen in the electrical resistivity, thermal conductivity, and heat capacity data; as well as (iii) *nodal character* of the superconducting state, established by means of thermal conductivity, heat capacity, NQR, magnetic penetration depth, INS and muon spin rotation/relaxation experiments. Most intriguingly, the compound seems to fulfill the necessary conditions for the formation of a modulated *Fulde-Ferrell-Larkin-Ovchinnikov* superconducting state, and therefore one might speculate on the emergence of this unique inhomogeneous phase at the low-temperature–high-magnetic-field corner of the $H-T$ phase diagram of $Ce_2PdIn_8$, as it possibly happens in the case of $CeCoIn_5$.

# Magnetic field induced charge rearrangement in magnetite and its relation to fast electronic processes

Z. Kąkol[1]

[1] *Wydzial Fizyki i Informatyki Stosowanej AGH, al. Mickiewicza 30, 30-059 Kraków*

Magnetite is the oldest magnet, the first Neel's test ground for his model of ferrimagnetism and the first material where the metal–insulator transition was suggested to undergo at $T_V = 124K$ in the so-called Verwey phase transition. But even now, after 70 years from the Verwey transition discovery, many aspects of this phenomenon should still be cleared. For example, the structure below $T_V$ was solved only recently and revealed subtle electronic structure in the form of trimeron lattice [1] that, according to yet another recent communication [2], may be switched within femtosecond range, i.e. the time by far surpassing all existing electronic devices. We review all those findings but also comment on our results on the magnetic and crystallographic axis switching process triggered by an external magnetic field. We show that although this process is best viewed by magnetization studies, it is also reflected in magnetostriction [3], causes some changes in electronic transport [4] and is altered when external pressure is exerted. We have also observed the axis switching microscopically by NMR that proved some electronic order alteration [5]. All those facts suggest that the axis switching process observed and studied by us is intimately linked with the fast change of electronic trimeron order mentioned above and reported in the recent literature [2].

[1] Charge order and three-site distortions in the Verwey structure of magnetite, M.S. Senn, J.P. Wright, and J.P. Attfield, Nature **481** (2012) 173

[2] Speed limit of the insulator–metal transition in magnetite, S. de Jong et al., Nature Materials, 2013 (10.1038/nmat3718)

[3] Magnetostriction of first and second order magnetite samples and its relation to the magnetic easy axis switching, A. Britwum et. al, Solid State Phenomena **194** (2013) 120

[4] Magnetoresistance in magnetite: Switching of the magnetic easy axis; G. Król et. al , Journal of Alloys and Compounds **480** (2009) 128

[5] Magnetically induced structural reorientation in magnetite studied by nuclear magnetic resonance, V. Chlan et. al, Journal of Applied Physics **108** (2010) 083914

## Superconductivity in intercalated iron chalcogenides

A. Krzton-Maziopa*[1], K. Conder[1], and E. Pomjakushina[1]

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Synthesis, crystal growth, structural and superconducting properties of the family of alkali metal (K, Rb, Cs) intercalated iron chalcogenides FeSe with Tc around 30K are reported. Single crystals have been grown by the Bridgman method. X-ray and neutron diffraction, micro x-ray fluorescence, magnetization and transport measurements have been applied to characterize the crystals. It was found that in the crystals two phases are coexisting - one majority magnetic phase and a diamagnetic minority phase, most probably, responsible for superconductivity. The phase separation was stated in our samples by means of the muon-spin rotation ($\mu$SR), neutron diffraction and High Resolution Electron Backscatter Diffraction.

Lithium doped chalcogenides have been obtained using pyridine as a solvent for a room temperature intercalation. We succeeded to obtain a new iron selenide superconductor with a $T_c$ onset of 45 K and the general formula $Li_x(C_5H_5N)_yFe_{2-z}Se_2$ (with x~0.8, y~0.05-0.2 and z~0.2) as both lithium and pyridine are intercalated into the structure.

* *Present address: Chair of Inorganic Chemistry and Solid State Technology, Warsaw University of Technology, Poland*

# New pnictide superconductor $Ln_4Fe_2As_2Te_{1-x}O_4$ (Ln=Pr, Sm, Gd) with $T_c$ up to 45 K.

J. Karpinski[1,2], S. Katrych[1], K. Rogacki[3], A. Pisoni[1], S. Weyeneth[4], S. Bosma[4], N. D. Zhigadlo[2], and L. Forro[1]

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[4] *Physik-Institut der Universität Zürich, 8057 Zurich, Switzerland*

In the frame of our studies new family of high $T_c$ pnictides superconductors has been discovered. Single crystals and polycrystalline samples of new superconductors $Ln_4Fe_2As_2Te_{1-x}O_4$ (Ln=Pr, Sm, Gd) have been grown under high pressure of 3 GPa at 1400-1500°C. In as grown undoped crystals $T_c$ = 25 K has been determined by magnetic and resistivity measurements. As result of fluorine doping $T_c$ of crystals or polycrystalline samples increased up to 45 K for $Gd_4Fe_2As_2Te_{1-x}O_{4-y}F_y$ and 40 K for $Sm_4Fe_2As_2Te_{1-x}O_{4-y}F_y$. The structure consists of the alternating $Fe_2As_2$ and $Pr_2O_2$ layers in the $c$ direction separated by tellurium atoms. It has close resemblance to the LnFeAsO structure. Lattice constants $a$ and $b$ are slightly larger (by ≈ 0.04 Å) while $c$ is considerably larger (by ≈ 21.3 Å). For Ln=Gd pnictogen height and As-Fe-As angle which are highly correlating with $T_c$, are 1.366(3) Å and 110.47(7)°, respectively. Te site reveals about 10 % of vacancies, which can be source of doping in as grown crystals without intentional doping.

S. Katrych et. al., Physical Review B **87**, 180508 (R) 2013.

## Manipulating magnetic anisotropy via the density of states at the Fermi level

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Magnetic anisotropy of ferromagnetic films ($FM$) is a key property for developing new technologies in spintronics. The magnetocrystalline anisotropy is caused by spin-orbit coupling of $d$-electrons. Thus, any manipulation of the $d$-electron bands, in particular if resulting in the change of occupied and/or unoccupied states close to the Fermi level ($E_F$), can lead to a significant increase of the anisotropy energy. The most striking example is the electronic structure altered at the surfaces and interfaces resulting in perpendicular easy magnetization axis of ultrathin films.

Another approach to modify the $d$-electron bands is related to the structural distortion realized by pseudomorphic growth of $FM$ films on mismatching substrates. For instance, in $Fe_{1-x}Co_x$ alloy films grown on mismatching $fcc-(001)$ substrates (like $Pd$, $Rh$ and $Ir$), modification of the electronic structure due to a strong tetragonal distortion, and adjustment of $E_F$ by $Fe-Co$ alloying, results in a strong perpendicular anisotropy [1].

If significant contributions to magnetic anisotropy are due to spin-polarized quantum well states ($QWS$) formed in the $d$-electron bands of $FM$ films, a similar effect can occur but only at specific thicknesses ($d_n = d_0 + nL, n = 1, 2, \dots$). The oscillation period $L$ is then determined by $k_{z0}$ (i.e. $k_z$ of the bulk $d$-band corresponding to $QWS$ that cross $E_F$) and can identify the electronic states which contribute to the anisotropy. The oscillation periods are different for $Co$ and $Fe$ films due to their different electronic structure and thus different $k_{z0}$ for the minority $d$-band electrons, which are responsible for the anisotropy oscillations in both cases [2].

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## Designing transition metal perovskites with favorable properties

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Transition metal oxides have been studied for several decades because of their intriguing properties resulting from strong coupling among crystal lattice and electron's orbital, charge and spin. In this talk I will review spectacular properties of $3d$ transition metal perovskites starting from ferroelectric titanates, through colossal magnetoresistive manganites, metal-insulator transitions in cobaltites and nicklates to superconductive cuprates. In recent years much has been learned about optimizing synthesis conditions and controlling structure-property relationships to design materials with novel or improved characteristics. I will describe our recent attempts to utilize this vast knowledge to develop new perovskites exhibiting multi-ferroic behavior and enhanced thermoelectric power. In addition, oxides display unique oxygen non-stoichiometry, which was used extensively to vary the valence state of transition metals and, as such, control the properties; for example, $T_c$ in $YBa_2Cu_3O_{7-d}$ or magnetic properties in $(Nd_{1-x}Ca_x)(Ba_{1-y}La_y)Co_2O_{5+d}$ systems. However, oxygen non-stoichiometry itself can be regarded as a useful property. I will show how the remarkable oxygen intake-release capability can be controlled in hexagonal manganites to devise new oxygen separation and storage materials.

# Evidence for multiple superconducting gaps in the filled skutterudite compound $LaRu_4As_{12}$

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Superconducting properties of the filled skutterudite compound $LaRu_4As_{12}$ [1] were investigated both as a function of temperature and magnetic field. At $T \ll T_c = 10.45\,\mathrm{K}$, the electronic contribution to the specific heat was found to be at variance with the predictions for an *s*-wave superconductor with one energy gap. In constant applied fields up to $H_{c2}(0) \approx 10.2\,\mathrm{T}$, multiple gaps have been further inferred from both a nonlinear magnetic-field dependence of the specific heat in the zero-temperature limit and a positive curvature of the upper critical field in the vicinity of $T_c$. Thus, $LaRu_4As_{12}$ appears to be a rare multiple-gap superconductor with cubic symmetry [2]. Most likely, its anomalous properties are associated with a spherical Fermi-surface sheet enclosing a small volume in the center of the Brillouin zone. Intriguing that evidence for multiband effects is observed in the compound with enhanced superconducting properties as compared to other skutterudite superconductors.

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## Disorder in Fe-based superconductors: effect on pinning and on pairing

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Disorder in type II superconductors provides pinning of vortex lines, but its pair-breaking effect limits critical temperature, $T_c$ . We investigated defect related properties of Fe-based superconductors (FBS) using two types of irradiation: heavy ion ( 6GeV Pb) to create correlated disorder and low temperature electron irradiation (2.5MeV at 20K) producing point like defects. Increase of irreversible magnetization and upward shift of irreversibility line, IRL was observed after heavy ion irradiation of all FBS investigated to date. Fingerprints of Bose-glass vortex state are revealed in heavy ion irradiated FBS crystals.Heavy ion irradiation does not depress $T_c$. In contrary, point-like disorder introduced by electron irradiation results in strong depression of $T_c$. In isovalently substituted $(Ba(FeAs_{1-x}P_x)_2$ crystals $T_c$ decreases linearly with dose down to 1/3 of initial value. An increase of normal state resistivity is observed and correlated with depression of $T_c$. Measurements of penetration depth $\lambda$ vs. temperature after incremental irradiation doses reveal changes of superconducting gap structure with disorder. In optimally doped $(Ba(FeAs_{1-x}P_x)_2$ linear $\lambda$ vs. T variation of pristine sample, indicative to nodes in gap, is observed. It becomes exponential, characteristic for fully gaped state after small irradiation dose. Further increase of disorder lead to $T^2$ variation of $\lambda$ expected for mid-gap states. This behaviour is incompatible with symmetry-imposed nodes of $d-wave$ pairing but consistent with $S^+/_-, S^+/_+$ mechanisms.

In collaboration with Takasada Shibauchi, Shigheru Kasahara and Yuta Mizukami, Kyoto University, Japon, Ruslan Prozorov, Makarii Tanatar, Ames Laboratory, Iowa, USA

## Peculiar magnetism of the FeAs – grand parent of the iron-based superconductors

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Iron mono-arsenide has been investigated by transmission $^{57}Fe$ Mössbauer spectroscopy in the temperature range 4.2–1000$K$. Additional spectra have been obtained at 20$K$ and 100$K$ applying external magnetic field of 7$T$[1]. Unusual anisotropy of magnetic hyperfine field on iron nuclei was discovered along the spin spiral versus orientation of the 3d magnetic moment. The anisotropy is due to the peculiarity of the $Fe$-$As$ bonds, the latter being of primary interest for iron-based superconductors. It was found that the spin spiral propagating along the $c$-axis leads to the complex variation of the hyperfine magnetic field amplitude with the spin orientation varying in the $a$-$b$ plane. Patterns are vastly different for iron located in the $[0\ k\ 0]$ positions and for iron in the $[0\ k+\frac{1}{2}\ 0]$ positions within the orthorhombic cell set to the *Pnma* symmetry. Lattice softens upon transition to the paramagnetic state at 69.2$K$ primarily in the $a$-$c$ plane as seen by iron atoms. This effect is quite large considering lack of the structural transition. Two previously mentioned iron sites are discernible in the paramagnetic region till 300$K$ by different electron densities on the iron nuclei. The anisotropy of the iron vibrations developed at the transition to the paramagnetic state increases with the temperature in accordance with the harmonic approximation, albeit tends to saturation at high temperatures indicating gradual onset of the quasi-harmonic conditions. It seems that neither hyperfine fields nor magnetic moments are correct order parameters in light of the determined static critical exponents.

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## Magnetism of the regular and excess iron in $Fe_{1+x}Te$ studied by Mössbauer spectroscopy

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The $Fe_{1+x}Te$ is a parent compound of the '11' iron-based superconductors and can be prepared by conventional solid-state method with excess iron $x$ = 0.04 – 0.18. Superconductivity with $T_c$ = 15$K$ under ambient pressure is induced by partial substitution of $Te$ by $Se$ or $S$. The magnetic ordering below 70$K$ for $Fe_{1+x}Te$ is complex as a result of competing interactions. Iron on the regular tetrahedral sites develops bicollinear antiferromagnetic structure for the almost stoichiometric compound, transforming into an incommensurate spin density wave (SDW) upon increasing $x$. The magnetic structure above $x \geq 0.12$ is interpreted as development of the elliptical helicity tending towards circular helicity for the highest $x$. The excess iron is located between regular $Fe$-$Te$ layers occupying partly available interstitials. The aim of this study is to understand how the amount of the excess (interstitial) iron affects the magnetic properties of the $Fe_{1+x}Te$.
$^{57}Fe$ Mössbauer spectroscopy was applied to investigate the $Fe_{1+x}Te$ for $x$ = 0.06, 0.10, 0.14, 0.18 within the temperature range 4.2$K$ – 300$K$ [1]. A spin density wave (SDW) within the iron atoms occupying regular tetrahedral sites was observed with the root mean square amplitude at 4.2$K$ varying between 9.7$T$ and 15.7$T$ with increasing $x$. Three additional magnetic spectral components appeared due to the interstitial iron. The excess iron showed hyperfine fields at approximately 16$T$, 21$T$ and 49$T$ for three respective components at 4.2$K$. Magnetic ordering of the interstitial iron disappears in accordance with the fallout of the SDW with the increasing temperature. Interstitial iron has relatively large localized magnetic moment at least for the site with the highest hyperfine field. These moments interact strongly with the electrons having ability to form Cooper pairs and prevent appearance of superconductivity. One has to remove this iron to have a chance to get superconducting material. Partial replacement of $Te$ by $Se$ or $S$ removes interstitial $Fe$ and one can get superconductor. Some minor components of the alcoholic beverages like weak organic acids remove excess $Fe$ as well. This work was supported by the National Science Center of Poland, Grant DEC-2011/03/B/ST3/00446.

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## The Fulde-Ferrell-Larkin-Ovchinnikov state in iron-pnictides

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The theoretical analysis of the Cooper pair susceptibility shows the two-band Fe-based superconductors (FeSC) support the existence of the phase with nonzero Cooper pair momentum (called the Fulde–Ferrel–Larkin–Ovchinnikov phase or shortly FFLO), regardless of the order parameter symmetry. Moreover this phase for the FeSC model with $s_{\pm}$ symmetry is the ground state of the system near the Pauli limit. [1] We discuss the $h-T$ phase diagram for FeSC in the two-band model and its physical consequences: the shape of the order parameter in real space and type of phase transitions.

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## Superconductivity of disordered Dirac fermions

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Recent discovery of topological insulators (TIs), a new class of materials that host topologically protected spin-helical Dirac surface states, launched the search for a topological superconducting analogue characterized by a fully gapped odd parity pairing state that could support Majorana bound states. Such a superconducting phase has important implications for a fault-tolerant quantum computing owing to the non-Abelian exchange statistics obeyed by Majorana fermions. Superconductivity reported thus far in some topological materials appears to be of bulk origin, with yet uncertain proximal connection to the topological Dirac fermion metal. In my talk I will discuss our most recent results on a 3D TI, $Sb_2Te_3$ synthesized under a modest pressure, where we have discovered nontrivial surface-like superconductivity with $T_c \sim 9$ K, the highest transition temperature among the TIs reported thus far. The diamagnetic state of this new superconductor is very unusual, since even in the normal state the system supports large orbital currents, while maintaining a robust singular spin response of the disordered Dirac fermions in the superconducting state. I will discuss our observations in the context of recent ideas of disorder assisted superconducting fluctuations that can turn Dirac semimetal into a superconductor.

## Breaking translational invariance by population imbalance: The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) states

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An overview is given of our present understanding of superconductivity with spontaneously broken translation symmetry in polarized Fermi systems. The existence of “crystalline" superconducting phases is considered in a wide range of systems, prominent examples being conduction electrons in metals, ultra-cold atoms in a trap, nuclear matter, and dense quark systems. The underlying physics is delineated and theoretical approaches to the inhomogeneous phases and their properties are discussed. From the experimental side it is argued that superconductivity with imbalance-induced order parameters is realized in layered organic compounds and potentially in heavy-fermion systems. Interesting phenomena are anticipated in (locally) non-centrosymmetric superconductors with strong spin-orbit interaction.

## Spin density wave states and phase separation in doped iron pnictides

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A possible mechanism of electronic phase separation in iron-based superconducting materials is proposed. It is based on the imperfect nesting of different portions of the Fermi surface in doped iron pnictides and chalcogenides. Similar approach [1] can be applied also to other materials with imperfect nesting, such as AA stacked graphene bilayer [2], chromium alloys, etc. We model the Fermi surface by two nearly circular hole pockets located near (0,0) point and two elliptically shaped electron pockets centered at $(0,\pi)$ and $(\pi,0)$ points. The ellipticity of the electron bands is characterized by parameter $\alpha$, where $\alpha = 0$ describes the circle and $\alpha \to \infty$ corresponds to the limit of infinitely thin ellipse. The coupling of charge carriers belonging to one electron and one hole bands by a weak electron-electron interactions leads to the formation of the commensurate spin-density wave (SDW) order. Upon doping. the commensurate SDW phase transforms to the incommensurate one. We show that in some doping range the ground state is unstable toward the electronic phase separation to the commensurate and incommensurate SDW phases with different charge carrier densities.

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## Disappearance of superconductivity in Fe-Te-Se system

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Fe-Te-Se system with simple crystallographic structure can be treated as a model system for investigations of the impact of magnetic impurities on superconductivity, since any substitution into antiferromagnetically ordered Fe-ions sublattice may eventually lead to appearance of localized magnetic moment. Early substitution studies strongly suggested that superconductivity in the system is closely related to the structural deformation rather than to the magnetic moment of the substituted ions. Two years ago, we have shown that only Co, Ni, and Cu ions are incorporated at the Fe site into the host lattice of the Fe-Te-Se single crystals and superconductivity disappears at the substitution level of few atomic percent. In the case of other dopants, inclusions, formed with elements not incorporated into the matrix, change the chemical composition of the crystals, leading to the changes in Se/Te ratio and the value of the critical temperature. Our recent results show very good correlation between decrease of superconducting volume fraction in Fe-Te-Se system and the amplitude of high-field Curie-type susceptibility. This indicates that, due to very short coherence length, the initial impact of localized magnetic moment introduced via substitutions into Fe-Te-Se system is a decrease of superconducting volume fraction without substantial reduction of the $T_c$ and only at the level of about 2 atomic percent of magnetic impurities concentration the superconductivity is completely suppressed. This allows to develop a system with coexisting superconducting and ferromagnetic stripe phases.

## Transition metal doping of FeSeTe: what can we learn from transport properties

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During recent years many studies have been devoted to probing superconductivity in the iron-based superconductors via impurity doping. Doping is a powerful tool used for tuning of material parameters: it may modify the density of carriers, the magnetic fluctuations, or the scattering rates. Many of these effects stem from the modifications of the Fermi surface topology. A nice example is the transition metal doped arsenic ferropnictide, $BaFe_2As_2$, which upon doping undergoes series of dramatic changes of the band structure, called Lifshitz transitions [1]. While these changes are best evidenced by the angle resolved photoemission spectroscopy, they also give signatures in the transport properties.

In this talk, after brief introduction on the transport in doped ferropnictides, I will discuss our recent transport investigations of the transition metal doped iron chalcogenide crystals, $FeTe_{0.65}Se_{0.35}$. So far very few attempts of successful doping have been described for this material. I will show that the evolution of the resistivity and the Hall effect up to high doping levels suggests that $FeTe_{0.65}Se_{0.35}$ may undergo changes of the band structure, possibly similar to those found in ferropnictides.

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## Crystal structure and physical properties of $NpPt_2In_7$ and $Np_2PdIn_8$

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The neptunium analogues of the $CePt_2In_7$ and $Ce_2PdIn_8$ layered intermetallic compounds have been synthesized and characterized by means of resistivity, magnetic susceptibility and heat capacity techniques. Rietveld analysis of the powder x-ray diffraction patterns of $NpPt_2In_7$ and $Np_2PdIn_8$ confirm tetragonal structure type for both compounds, with lattice parameters similar to those previously reported for $CePt_2In_7$ and $Ce_2PdIn_8$, respectively.

For $NpPt_2In_7$ an antiferromagnetic transition was observed with the Néel temperature $T_N$=23 K. Rather complex magnetism is revealed for $Np_2PdIn_8$ with ferromagnetic and possibly antiferromagnetic transitions at $T_C$=9.5 K and $T_N$=8.5 K, respectively. For both $NpPt_2In_7$ and $Np_2PdIn_8$ a Curie-Weiss fit of the high-temperature magnetic susceptibility curve, $\chi(T)$, gives an effective magnetic moment as expected for trivalent Np.

First-principles electronic structure calculations based on the local spin density plus Coulomb interaction and the local density plus "Exact Diagonalization" approximations are used for theoretical investigation of the electronic and magnetic character of $NpPt_2In_7$, and compared to the experimental findings.

## Nanostructures with highly controllable electronic properties

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Combined quantum structures which can be steered from the outside are highly relevant to new technologies in which the control and manipulations of electron spin and wave functions play an important role. We have considered quantum nanostructures [1,2] composed of a semiconductor quantum dot surrounded by a quantum ring. The properties of such nanostructures can be strongly modified by changing the shape and the height of the barrier separating the structure and/or the relative position of the minima of the potential wells. The manipulation of these parameters by, e.g., electrical gating leads to the change of the shape and the radial distribution of wave functions which strongly influence many properties. We have shown that such wave function engineering can alter:

a) the relaxation time of a nanostructure used as spin qubit or memory device by orders of magnitude,

b) the cross-section for intraband infrared or microwave absorption from large to negligible,

c) the conducting properties of arrays of dot-ring nanostructures from highly conducting to insulating.

We have also shown that a dot-ring nanostructure exhibits features of single electron transistor and electrical current rectifier.

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## Non-Abelian anyon statistics arising from pairing of composite fermions in fractional quantum Hall effect

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Convincing demonstration of non-Abelian anyon quantum statistics, corresponding to a multi-dimensional realization of the braid group, remains a major challenge in contemporary condensed matter physics. The physical system relevant for this quest is a two-dimensional electron gas in a high magnetic field, condensing into a quantum liquid and exhibiting fractional quantum Hall (FQH) effect. The understanding of electron correlations in the FQH regime relies on the formation of "composite fermions" (electrons binding vortices of the many-body wave function). At the particular Landau level filling factor (defined as the number of electrons per magnetic flux quantum $hc/e$) of $\nu = 5/2$, composite fermions experience a vanishing effective magnetic field and are believed to form a condensed $p$-wave paired state. Elementary excitations of this hypothetical liquid have fractional charge $\pm e/4$ and non-Abelian statistics, corresponding to the Ising model with two degenerate fusion channels. I will present evidence for the above scenario coming from various numerical calculations. In particular, I will discuss ferromagnetism and skyrmions [PRL 104, 086801 (2010)], quasiparticles and their topological degeneracy [PRL 107, 086806 (2011)], and the counting and dispersion of neutral collective modes [PRL 107, 036803 (2011); PRL 107, 136802 (2011)], all consistent with composite fermion pairing. Other FQH states with more complicated braiding properties will also be invoked, and a simple unifying picture of non-interacting composite fermions with additional discrete degree of freedom will be drawn [PRB 87, 245125 (2012)].

## Nonequilibrium propagation of single holes and bound pairs in the t-J model

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We perform an accurate time–dependent numerical study to investigate out–of–equilibrium response of a single hole and a bound state within $t$–$J$ systems on a two–leg ladder and a square lattice. Since the system is subjected to a uniform electric field, the only dissipation mechanism which leads to a finite steady current is the emission of spin excitations. We show that the bound state decays with the onset of finite steady current if both mechanisms for binding and the dissipation share matching degrees of freedom [1]. Moreover, by investigating the mechanism of decay on the square lattice we find that the dynamics is governed by the decay in the direction perpendicular to the electric field, leading to much shorter decay times in comparison to the ladder where such dynamics is topologically restricted.

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## Linear-response dynamics from the time-dependent Gutzwiller approximation

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In this presentation we introduce a time-dependent Gutzwiller approximation (TDGA) for general multi-band Hubbard models [1]. Our approach generalises earlier ideas for a TDGA by explicitly incorporating the coupling between time-dependent variational parameters and a time-dependent density matrix. From the time-dependence of these quantities we obtain dynamical correlation functions in the linear-response regime. As a a first application we apply our method to the one-band model where we show that the interacting system can be mapped to an effective problem of fermionic quasiparticles coupled to 'doublon' (double occupancy) bosonic fluctuations. The latter have an energy on the scale of the on-site Hubbard repulsion $U$ in the dilute limit but becomes soft at the Brinkman-Rice metal insulator transition.

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## Superconductivity in the two-dimensional Hubbard model: Gutzwiller wave function solution

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A systematic diagrammatic expansion for Gutzwiller-wave functions (DE-GWF) is formulated [1] and used for the description of superconducting (SC) ground state in the two-dimensional Hubbard model with electron-transfer amplitudes $t$ (and $t'$) between nearest (and next-nearest) neighbors. The method is numerically very efficient and allows for a detailed analysis of the phase diagram as a function of all relevant parameters ($U$, $\delta$, $t'$). SC states appear only for substantial interactions, $U/t > 3$, and for not too large hole doping, $\delta < 0.32$ for $t' = 0.25t$; this upper critical doping value agrees well with experiment for the cuprate high-temperature superconductors. We also obtain other important and novel features of the SC state: (i) the SC gap at the Fermi surface resembles $d_{x^2-y^2}$-wave only around the optimal doping and the corrections to this state are shown to arise from the longer range of the pairing; (ii) the nodal Fermi velocity is almost constant as a function of doping and agrees quantitatively with the experimental results; (iii) the SC transition is driven by the kinetic-energy lowering for low doping and strong interactions. We compare our results with those of the variational Monte Carlo method. The work was supported by the Foundation for Polish Science (FNP) under the 'TEAM' program, as well as by the project 'MAESTRO' from National Science Centre (NCN), No. DEC-2012/04/A/ST3/003420.

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# Even parity spin-triplet pairing induced by the combined effect of the Hund's rule and correlations in two-band Hubbard model

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Spin-triplet superconductivity is believed to appear in $Sr_2RuO_4$, $UGe_2$, URhGe, and UIr. In the last three compounds the paired phase coexists with ferromagnetim, whereas in $UNi_2Al_3$ and $UPt_3$, the coexistence with antiferromagnetism has been observed. The question of the microscopic mechanism that induces the spin-triplet paired phase still remains open. Here we analyze [1,2] the universal aspects of the Hund's-rule induced spin-triplet pairing within the two-band Hubbard model on a square lattice. According to our calculations, this pairing mechanism, in conjunction with the correlation effect, can lead to pure superconducting states, as well as coexistent with magnetic ordering. Furthermore, even though all the interactions in the considered model are of intraatomic character, the pairing contains both intra- and inter-site components. It should be emphasized that this model is not as yet material specific. However, it allows for the analysis of general features of the proposed pairing mechanism. The calculations have been carried out with the use of the so-called *statistically consistent Gutzwiller approximation.*

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## d-wave superconductivity and its coexistence with antiferromagnetism in t-J-U model: Statistically consistent Gutzwiller approach

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We discuss the *t-J-U* model using the so-called statistically-consistent Gutzwiller approximation (SGA). The coexistence of antiferromagnetism and d-wave superconductivity is examined in $T \to 0$ limit; we show[1] that such consistency appears only for $U/|t| \gtrsim 10$ and in a very narrow range of doping ($\delta < 0.006$) in the vicinity of the Mott insulating state, in contrast to some previous reports. The dependence of optimal doping on value of $J$ is presented. Additionally, the effect of hopping to the second nearest neighbors is discussed, as well as the extension to $T \neq 0$ case.
The work was supported by the Foundation for Polish Science (FNP) under the 'TEAM' program, as well as by the project 'MAESTRO' from National Science Centre (NCN), No. DEC-2012/04/A/ST3/003420.

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## Imaging vortices in superconductors with very low temperature scanning tunneling microscopy and spectroscopy

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The observation of vortices in superconductors was a major breakthrough in developing the conceptual background for superconducting applications. Each vortex carries a flux quantum, and the magnetic field radially decreases from the center. Techniques used to make magnetic field maps, such as magnetic decoration, give vortex lattice images in a variety of systems. However, strong type II superconductors allow penetration of the magnetic field over large distances, of order of the magnetic penetration depth. Superconductivity survives up to magnetic fields where, for imaging purposes, there is no magnetic contrast at all. Reciprocal space studies using neutron scattering have been employed to obtain insight into the collective behavior. But the microscopic details of vortex arrangements and their motion remain difficult to obtain. Direct real space visualization can be made using scanning tunneling microscopy and spectroscopy. Instead of using magnetic contrast, the electronic density of states describes spatial variations of the quasiparticle and pair wavefunction properties. This occur at distances of order of the superconducting coherence length, which is much smaller than the magnetic penetration depth. I will discuss recent advances in vortex imaging made with scanning tunneling microscopy and spectroscopy. Vortex images reveal the influence of the Fermi surface distribution of the superconducting gap on the internal structure of vortices. Current driven imaging opens new perspectives, both in the understanding of vortex cores and the dynamics of the vortex lattice.

## On strontium ruthenate enigma

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Strontium ruthenate is an interesting system with a Fermi liquid like normal state at low temperatures and a very anomalous superconducting state. It has been proposed as a spin triplet odd parity superconductor. Unfortunately 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 a gap vanishing somewhere on the Fermi surface. The T independent spin susceptibilities measured with a magnetic field in the *ab* plane and along the c-axis are at odds with the theory which requires one of the components to change with temperature. The temperature dependence of the nuclear spin relaxation rates $1/T_1$, measured for various nuclei, show conflicting results. The material shares the puzzling existence of an orbital moment with $^3He$ - the spin triplet superfluid analogue. A naive estimate would predict a magnetisation comparable to ferromagnetic iron. However, yet no sign of magnetic fields at the boundaries or near defects has been observed again in complete disagreement with theoretical predictions. The theoretical interpretation of the Kerr effect, another hallmark of time reversal symmetry breaking is also challenging. All these issue rise a number of fundamental questions. We will discuss the model which takes into account the three relevant orbitals and the three dimensionality of the system and is able to describe semi-quantitatively a number of these puzzling properties of the material.

## Inverse proximity effect in hybrid organic-inorganic systems

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Superconducting properties of thin Nb films covered with self assembled molecular layers (SAM), linking films to 5 or 10 nm gold nanoparticles attached to the molecules heads, have been investigated. The critical temperature $T_C$ of the films was found to change upon attachment of gold nanoparticles to the linker molecules. Surprisingly, $T_C$ is routinely enhanced when SAM of 3 nm long diSilane are used, whereas deposition of shorter linkers causes either classical proximity-like reduction of $T_C$ or its enhancement. No change in critical temperature have been observed when gold nanoparticles are only physisorbed on a layer of organic molecules or low transparency molecules are used. Simultaneously to the critical temperature enhancement a significant increase in critical currents of decorated Nb films have been observed. However, deposition of bare molecules have not influenced neither the critical temperature not the critical current of the films. Tunneling spectra acquired on the linked gold nano particles below $T_C$ typically exhibit zero-bias peaks, and occasionally, for the shorter linkers only, also a gap in the density of states. The observed effects can be accounted for by a new pairing mechanism involving a coupling between electrons from gold nanoparticles and Nb film, mediated by the vibrations of the organic linker molecules. Preliminary experiments show appearance of similar $T_C$ enhancement effects in high-$T_C$ LSCO films covered with medium length molecules and Au nanoparticles.

## Odd-frequency spin triplet pairing correlations in ferromagnet/superconductor multilayer systems

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In heterostructures with magnetic and superconducting layers a number of novel proximity effect phenomena occur. Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) like oscillations been observed in oscillating normal and $\pi$-Josephson junction behaviour in S/F/S multilayer structures. The breaking of inversion symmetry also leads to pairing correlations in the $S = 1$, $S_z = 0$ triplet channel. In addition, if non-colinear magnetic materials (eg holmium) are included, then pairing correlations occur in the $S = 1$, $S_z = \pm 1$ triplet channels. These generate a long ranged proximity effect (Robinson Witt and Blamire, Science **329** 59-61 (2010)). We present microscopic calculations of the pairing correlations in these structures and confirm that the pairing correlations are retarded in time (odd frequency). We explore in detail the effect of the holmium layers, and examine triplet pairing correlations as a function of thickness and magnetic geometry of the holmium.

## Holes in an antiferromagnet: Monte Carlo studies of the Ising t-J model

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Using recently developed approach to the $t$-$J$ model some of its features are analyzed. In particular, we study the destruction of the antiferromagnetic (AF) order by doping [1] and the interplay between the AF order and hole mobility. In some circumstances this competition may lead to formation of ferromagnetic polarons in AF background [2]. The advantage of the proposed method is that large systems up to a few hundred lattice sites can be easily studied by means of a modified classical Monte Carlo technique [3]. It is particularly important in the small-$J$ regime, where the size of the polaron is large. This is the regime which is not accessible by the Quantum Monte Carlo and Lanczös methods.

For one and a few holes we calculate how the size of the ferromagnetic polaron depends on $J$. We show that the results obtained for the so-called Ising $t$-$J$ model are consistent with the exact digonalization studies for the $t$-$J$ model [4], but allows to analyze this model for much smaller $J$. We also demonstrate that in this regime a phase separation occurs for a finite concentration of holes.

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## Spectral function of the anomalous propagator

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We argue that in order to unambiguously identify the pairing mechanism in complex superconductors such as the cuprates, a detailed study of the spectral function of the anomalous propagator may be useful. We present exact sum rules for a few moments of such spectral functions, as obtained within the Eliashberg theory and for the repulsive Hubbard model, which is believed to exhibit d-wave superconductivity. We conclude by discussing the experimental observability of the spectral function of the anomalous propagator.

## Unified character of electron correlation effects in unconventional Pu-based superconductors and $\delta$-Pu

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Electronic structure calculations combining the local density approximation with an exact diagonalization of the Anderson impurity model show intermediate $5f^5$-$5f^6$-valence ground state and delocalization of the $5f^5$ multiplet of the Pu atom $5f$-shell in $PuCoIn_5$, $PuCoGa_5$, and $\delta$-Pu. The $5f$-local magnetic moment is compensated by a moment formed in the surrounding cloud of conduction electrons. For $PuCoGa_5$ and $\delta$-Pu the compensation is complete and the Anderson impurity ground state is a singlet. For $PuCoIn_5$ the compensation is partial and the Pu ground state is magnetic. On the basis of these results, we suggest that unconventional $d$-wave superconductivity is likely mediated by the $5f$-states antiferromagnetic fluctuations in $PuCoIn_5$, and by valence fluctuations in $PuCoGa_5$.

## Strain and substitution effects on electronic structure of iron selenide superconductors

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The influence of different kinds of strain on both crystal and electronic structures of FeSe [1] and $FeSe_{0.5}Te_{0.5}$ [2] superconductors as well as of doping with S, Te, Co, Ni and Cu atoms [3] have been investigated employing various DFT methods: FPLO, Abinit, Quantum Espresso. We focused mainly on changes in the Fermi surface (FS) nesting between the holelike and electronlike corrugated cylinders as crucial for rising unconventional superconductivity, in particular mediated by spin fluctuations (SF). Our calculation results are in good accord with former experimental data and support the nesting scenario of superconductivity in these iron chalcogenides.

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# Effect of tetragonal distortion on the electronic structure, phonons and superconductivity in $Mo_3Sb_7$

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A Zintl-type compound $Mo_3Sb_7$ has gained much attention in recent years due to its interesting superconducting ($T_c \simeq 2.2$ K, Bukowski *et al.* 2002) and transport properties. Candolfi *et al.* (2007) suggested that spin fluctuations compete with superconductivity in this compound. Later on, Tran *et al.* (2008) suggested an AFM spin dimer formation below $T^* = 50$ K. Next, Koyama *et al.* (2008) observed a structural cubic-to-tetragonal transition below $T^* = 53$ K, driven by the frustration in antiferromagnetic interactions. Recently, structural parameters of the tetragonal phase were determined for the first time (Yan *et al.*, 2013). This prompted us to reinvestigate the electronic structure, dynamical properties and electron-phonon interaction in the tetragonal $Mo_3Sb_7$ to discuss the effect of crystal deformation on the aforementioned characteristics. Our results show, that tetragonal distortion has small, but positive effect on superconductivity, slightly increasing electron-phonon coupling constant $\lambda$. This supports our earlier conclusion, drawn for the cubic phase (Wiendlocha *et al.*, 2008) that the electron-phonon mechanism is likely to be responsible for the superconductivity in $Mo_3Sb_7$. Moreover we point out that the tetragonal distortion transforms $Mo_3Sb_7$ into the noncentrosymmetric superconductor, which was surprisingly previously overlooked. This observation opens new possibilities for the superconducting pairing symmetry in this compound. In this context, we discuss the influence of the spin-orbit interaction on the electronic structure of $Mo_3Sb_7$.

# Phase diagram of $d$-wave superconductors with charge density waves and stationary Josephson current in junctions made of such materials

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The phase diagram of $d$-wave superconductors partially gapped by biaxial or unidirectional charge density waves (CDWs) was considered. The model was applied to cuprates. It was shown that the temperature, $T$, dependence of the CDW order parameter $\Sigma$ is reentrant in a certain region of phase diagram $\sigma_0 - \alpha$, where $\sigma_0$ is the ratio between the electron-hole and Cooper pairing strengths and $2\alpha$ is the width of the CDW sector in the momentum plane. The stationary Josephson tunnel current $I_c$ was calculated for junctions made of such superconductors. The directionality of tunneling was made allowance for. In all studied cases, the dependences of $I_c$ on the angle $\gamma$ between the chosen crystal direction and the normal to the junction plane were found to be significantly influenced by CDWs. The results testify that the orientation-dependent patterns $I_c(\gamma)$ measured for CDW superconductors allow the CDW configuration (unidirectional or checkerboard) and the symmetry of superconducting order parameter to be determined. It was shown that when CDWs are absent or weak, there exists an approximate proportionality between $I_c(x)$ and the product of superconducting energy gaps $\Delta(x)$ and $\Delta(x')$ on both sides of the tunnel barrier (the law of corresponding states, LCS). Here, $x$ is either the reduced temperature, $T/T_c$, where $T_c$ is the superconductor critical temperature, or one of the problem parameters ($\sigma_0$ and $\alpha$). However, for a high directionality of tunneling and special experimental setups, CDWs may violate the LCS. The proposed method can be used to reveal CDWs in cuprates.

# Coexistence of superconductivity and ferromagnetism in $Y_9Co_7$: a renewed experimental study

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Physical properties of $Y_9Co_7$ have been reinvestigated utilizing resistivity, magnetization and specific heat measurements made by modern experimental techniques applied to a carefully-selected chemically-homogeneous polycrystalline specimen. Solid evidence for the superconductivity below $T_{sc} \approx 2.95K$ and the weak itinerant ferromagnetism below $T_C \approx 4.5K$ has been found in both the transport and thermodynamic quantities. In addition to the largest value of $T_{sc}$ ever reported, we observed a clear reduction of the electronic contribution to the heat capacity in the superconducting state suggestive of the lower entropy than in the normal state as well as a substantial enhancement of the upper critical field. The microscopic properties of the ferromagnetic state point at the interplay of both superconductivity and ferromagnetism on a microscopic scale in $Y_9Co_7$, as opposite to some believe that the superconducting state occurs in the paramagnetic phase. When combined with the recent observation e.g. for $UGe_2$ and $UCoGe$ systems, our results support an expectation that metallic ferromagnets may universally become superconducting for a special crystal structures and when the magnetization is small. Our understanding of coexistence of superconductivity and the weak itinerant ferromagnetism of $Y_9Co_7$ will be presented also on the basis of previous experimental results [1,2] as well as the band structure calculations [3].

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## Band magnetism with inter-site correlations and interactions

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New decouplings are proposed for the Hubbard model, which include the inter-site kinetic correlation and the hopping interaction. Hopping interaction is the result of the occupationally dependent hopping integral. It is responsible for the bandwidth change and also contributes to the exchange field.

The impact of these new physical factors on the band ferromagnetism and antiferromagnetism is reviewed. Comparison with the results of previous CP approximation is included.

# Crystal-field interactions in $RPd_2Al_3$ intermetallics (R = Pr, Nd, Sm and U)

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We have analyzed crystal-field (CEF) interactions in series of intermetallics $PrPd_2Al_3$, $NdPd_2Al_3$, $UPd_2Al_3$, being strongly motivated by a recent claim for *ab-initio*, using the GGA form for the exchange potential, calculations of CEF parameters for $SmPd_2Al_3$ (Phys. Rev. **81** (2010) 024413). The interest to this series of compounds has started in 1991 with discovery by Prof. Steglich of the superconductivity in $UPd_2Al_3$ ($T_{sc}$ = 2 K) coexisting with the antiferromagnetic state below $T_N$ of 14 K. Apart of the surprising superconductivity there was long debate on the role played by $f$ electrons, they are itinerant or localized, and about a number, two or three, of localized $f$ electrons. We have succeeded in description of the inelastic-neutron-scattering spectra i.e. of the $U^{3+}$ ion in $UPd_2Al_3$. This trivalent state is supported by recent observation of the $Sm^{3+}$ state in isostructural $SmPd_2Al_3$. The derived set of CEF coefficients explains, for instance, the nonmagnetic ground state of $PrPd_2Al_3$, the easy magnetic hexagonal plane for $NdPd_2Al_3$ and $UPd_2Al_3$, and the easy magnetic c-axis for $SmPd_2Al_3$ and $NpPd_2Al_3$. Within the Quantum Atomistic Solid State theory (QUASST) we consistently have explained the ground-state properties and thermodynamics, both in the paramagnetic and magnetic state, together with the reproduction of the $\lambda$-type peak at the magnetic phase transition. Our studies indicate that 1) the crystal field exists in these intermetallics and that 2) in all discussed intermetallics the rare earth or U ions are in the trivalent state.

## Evolution from a magnetically correlated state to a single impurity state in heavy fermion system $Ce_{3-x}La_xCo_4Sn_{13}$

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$Ce_3Co_4Sn_{13}$ crystallizes in the cubic $Yb_3Rh_4Sn_{13}$ structure, which is closely related to the one of scutterudites, well known thermoelectric materials. $Ce_3Co_4Sn_{13}$ exhibits novel physical properties, a large increase in $C_{mag}/T$ was recently observed at low temperatures with a maximum value of about 4 $J/K^2mol_{Ce}$. The specific heat data suggested that $Ce_3Co_4Sn_{13}$ is likely near a magnetic quantum critical point (QCP). To investigate this idea further, we measured a low-temperature specific heat and magnetic and electronic transport properties of $Ce_{3-x}La_xCo_4Sn_{13}$ in order to study the proximity of $Ce_3Co_4Sn_{13}$ to the possible magnetic QCP. We found the critical concentration $x_c \approx 0.6$ which separates the magnetically correlated state with a maximum in $C(T)/T$ at $\sim$ 0.7 K for $x < x_c$, and a single impurity state for $x > x_c$ in heavy fermion (HF) system $Ce_{3-x}La_xCo_4Sn_{13}$. However, for $x_c$ the low-temperature $C(T)/T$ and magnetoresistivity $\rho(T, B)$ behaviours are not characteristic of the QCP. We also present the low-temperature properties of the reference $La_3Co_4Sn_{13}$, which exhibits a superconductivity below $T_C \sim 3$ K and unusual behaviour of $T_C$ under external pressure.

## A Hund's rule stabilized magnetic nematic phase in $URu_2Si_2$?

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The underscreened Anderson Lattice Model with spin-rotational interactions can exhibit a novel second-order phase transition that is driven by the spin-flip terms of the Hund's rule exchange interaction[1]. The interaction produces a spin-dependent mixing of 5f bands with differing orbital characters. The resulting orbital density wave for the spin-up electrons is compensated by an orbital density wave for the down-spin electrons. The transition breaks spin-rotational invariance but does not lead to a net staggered magnetic moment. In particular, it does produce an anisotropy in the magnetic susceptibility similar to that reported for $URu_2Si_2$ [2]. Since the model gaps most of the Fermi-surface, and since the order-parameter is difficult to observe, the model might describe the "Hidden Order" phase of $URu_2Si_2$. We examine a magnetic nematicity which develops belwo teh Hidden Order transition.

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## Scanning tunneling microscopy and spectroscopy of superconducting molybdene carbide ultra thin films

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Studies on strongly disordered superconductors can help understanding the superconductor-insulator transition. We study the MoC superconducting films where an increase of disorder and suppression of the superconducting transition temperature is achieved by depleting their thickness down to 5 nm. $T_c$ equals to 8.32 K for the bulk material. Using scanning tunneling microscopy and spectroscopy (STM/S) below 1 K we addressed the topography and spectral maps of the superconducting density of states (SDOS) on the films with 10 nm and 5 nm thickness, with $T_c$ = 6 and 4 K, respectively. The thicker film shows a BCS-like SDOS but with a significant broadening. Strong deviations from BCS-like characteristics are found on the 5 nm film. The results are discussed in the context of the STM/S measurements published on other disordered superconductors close to the superconductor-insulator transition.

## Superconductivity in $\gamma$-U alloys

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Uranium metal, know at room temperature in its orthorhombic a phase, was traditionally considered as a superconductor with critical temperature below 1 K. Only recently it was found that the best single crystals are actually non-superconducting [1]. They fully develop a CDW state below 38 K, which is contra-indicative for superconductivity. SC observed in normal bulk U is related to defected areas like grain boundaries, which do not allow to develop the CDW state. A special soft phonon mode existing in the orthorhombic structure has been considered the source of *e-ph* coupling [2]. On the other hand, there exist old reports that the *bcc* phase of U ($\gamma$-U) stabilized to low $T$ by doping, exhibits superconductivity, too [3]. We have been studying properties of U-Mo alloys, which were prepared in the *bcc* structure with the aid of ultrafast cooling, allowing to reduce the Mo concentration, necessary to provide pure *bcc* structure, down to 11 at.%. The critical temperature reaches 2.1 K for 15% Mo. The most striking feature (for such low $T_c$) is the very high upper critical field $\mu_0 H_{c2}(0)$, estimated as 5-7 T. This makes a clear distinction to the $\alpha$-U superconductivity, which is suppressed in $\approx$ 0.3 T. We tentatively classify the alloys as strongly coupled BCS superconductors.

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## 'To screen or not to screen, That is the question': Kondo impurity on interface with superconductor

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Spinful impurities immersed in the bulk materials are known to have a detrimental influence on the otherwise clean superconducting systems, either by breaking the electron pairs or restricting (in space) their long range coherence. Recently, however, a different aspect attracts considerable amount of interests. It is related to the following question: how does the macroscopic superconducting reservoir affect the spinful impurity once they are brought in a contact.

Since the proximity effect spreads electron pairing onto the quantum impurity (converting it into a superconducting grain) the true eigen-states are represented by linear combinations of the empty and doubly occupied configurations $u\,|0\rangle + v\,|\uparrow\downarrow\rangle$. Whether such BCS-type states are energetically preferable over the singly occupied configurations $|\uparrow\rangle$, $|\downarrow\rangle$ depends on interplay between the Coulomb potential $U$, the proximity-induced gap $\Delta_d$ and initial energy level $\varepsilon_d$ of the quantum impurity. In nanoscopic junctions these parameters can be varied at will, thereby enabling observation of the quantum phase transitions from the Kondo to the BCS state (or vice versa) in a controllable manner [R. Maurand, Ch. Schönenberger, Physics **6**, 75 (20013)]. I shall address these and similar issues referring to the theoretical studies and the recent experimental realizations.

## Seebeck effect in the graphene – superconductor junction

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Thermopower of graphene-superconductor (GS) junction is analyzed within the extended Blonder-Tinkham-Klapwijk formalism. Within this approach, we have also calculated the temperature dependence of the zero-bias conductance for GS junction. Both quantities reflect quasi-relativistic nature of massless Dirac fermions in graphene. Both the linear and the non-linear regimes are considered.
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## Indirect RKKY interaction in graphene nanoflakes

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Graphene nanoflakes exhibit a number of interesting properties. Their nontrivial magnetic characteristics include the form of an indirect Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between localized magnetic moments in such nanostructures.

In the paper the results of non-perturbative calculations of indirect RKKY coupling in graphene nanoflakes (quantum dots) are presented [1]. Various shapes and edge forms (armchair or zigzag edge) as well as different nanostructure sizes are considered. Basing on the tight-binding real space Hamiltonian for charge carriers in a finite system, supplemented with the Hubbard term treated in Mean Field Approximation, the exchange energy is derived from the total energy of the system [1-3]. The importance of the coulombic interactions in such calculations is underlined. The influence of charge doping on the indirect coupling is particularly emphasized in the study. Moreover, in finite systems, an additional indirect coupling mechanism, similar to double exchange, may emerge due to the states filled with single electrons.

This work has been supported by Polish Ministry of Science and Higher Education on a special purpose grant to fund the research and development activities and tasks associated with them, serving the development of young scientists and doctoral students. The computational support on HUGO cluster, P. J. Šafárik University in Košice is gratefully acknowledged.

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# Kondo resonance in $Ce_2CoSi_3$ studied by angle resolved photoemission spectroscopy

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A nonmagnetic Kondo lattice $Ce_2CoSi_3$ is a promising system for studies of hybridization based on a Kondo interaction. The Kondo and coherence temperatures are relatively high and the first estimates indicate that they are of the order of 50 K and 80 K respectively. The electronic specific heat amounts to $C/T$=200 mJ/(mol$_{Ce}$K$^2$) at T=0.4 K.

Angle resolved photoemission spectroscopy studies on $Ce_2CoSi_3$ revealed a band structure along [0001] crystallographic direction. The spectra are dominated by a high intensity parabolic band of surface origin and an electron pocket around the Γ point, which is related to bulk. The experimental data are compared to the calculations obtained by means of the full-potential local-orbital (FPLO) code with LSDA+U approach. A considerable variation of the quasiparticle weight in a Kondo peak along the Fermi surface is observed. It points to the existence of a high anisotropy of the hybridization between 4f and conduction band electrons.

## Perspectives for ultra-low temperature research at the Academic Center of Materials and Nanotechnology at AGH in Krakow

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We take the opportunity to advertise a newly built ultra low temperature laboratory at the Academic Center of Materials and Nanotechnology at AGH University of Science and Technology in Krakow. The laboratory's main strength rests upon a dry i.e. cryogen-free dilution refrigerator capable of achieving temperatures as low as 9mK in the presence of external magnetic fields of up to $\mu_0$H=9T. Future work into unconventional superconductivity, topological insulators, graphene and the technology of achieving micro-Kelvin temperatures will be briefly outlined in the presentation. Anyone interested in collaborating is welcome to get in touch!

## Hysteresis of magnetic moment of superconducting Nb and Ta cylinders

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Magnetic irreversibility of flux penetration was experimentally investigated in superconducting Nb (k=$\lambda/\xi$=1,28, $\lambda$- depth of penetration, $\xi$- coherent length) and Ta (k=$\lambda/\xi$=0,38) cylinders (with relations of height/diameter $(h/d)_{Nb}$=6, $(h/d)_{Ta}$=4,7; d=3mm). High-purity metal samples (for Nb $\rho_{300}/\rho_{10}$ ~1500) were annealed during 2 hours at T=2300 C in order to lower the pinning. Squid magnetic moment measurement shows strongly irreversible behavior at remagnetization in the magnetic fields $H_{c1g} < H \leq H_{c2}$, where $H_{c1g}$ is the magnetic field of magnetic flux entrance and $H_{c2}$ is the second critical field. The experimental data shows that the first penetration field into sample is considerably lower than first critical field $H_{c1}$. The temperature dependencies of different characteristic fields ($H_{c1g}$, $H_{c1}$, $H_{c2}$) were investigated. All specimen shapes (apart from ellipsoid) exhibit magnetic irreversibility due to a geometric barrier for flux penetration [1]. This is true for both type I [2] and type II [3, 4] superconductors. The role of geometric barrier, surface barrier and pining in magnetic irreversibility of flux penetration into superconducting cylinders Nb and Ta were discussed taking into account results of investigation in [5,6]. Here we compare the irreversible magnetization loops of cylinders for two orientations of magnetic field: along and perpendicular to the axis. We also try to calculate the irreversible magnetic properties of superconducting cylinders for these two sample orientations.

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## Application of ALPS 2.1.1 for simulations in strongly correlated systems

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The latest version of ALPS project (*Algorithms and Libraries for Physics Simulations*) and its application in theory of strongly correlated systems will be presented[1]. ALPS is an open source software developed since 2004 by theoretical physicists working in the field of condensed matter physics[2]. The ready-made applications are implmentation of the most important algorithms for lattice models, such as classical and quantum Monte Carlo (MC, QMC) in the local and cluster update version, quantum Wang-Landau method (QWL), sparse and full diagonalization (Lanczos, ED), Density Matrix Renormalization Group (DMRG), Dynamic Mean Field Theory solver (DMFT) and Time-Evolving Block Decimation (TEBD). At a basic level, simulations and numerical computations do not require any programming knowledge in *C++* language (the main libraries and applications). The package uses a common input/output *XML* data format to describe lattices, models and parameters. Open source is, however, a framework to develop their own software using parallel computing (open-MPI) on different platforms. The version 2 of ALPS offers the HDF5 standard to store and organize large amounts of numerical data, the new specialized programs for performance analysis (written in *Python*) and uses the workflow system *VisTrails* to manage and visualization of computational processes. The simplest version of the system *liveALPS* will be also presented.

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## Exotic spin orders driven by orbital fluctuations in the Kugel-Khomskii model

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Spin-orbital entanglement in Mott insulators with active orbital degrees of freedom has important consequences for the ground and excited states [1]. We have studied phase diagrams by varying crystal-field splitting and Hund's exchange in the two-dimensional (2D) square lattice and three-dimensional (3D) cubic Kugel-Khomski model, using the cluster mean field theory and the entanglement renormalization ansatz. When $3z^2 - r^2$ orbitals are favored by the crystal field in the 2D model, both methods give a non-collinear exotic magnetic order when antiferromagnetic (AF) and ferromagnetic (FM) interactions compete [2]. In the 3D model we identify three phases with exotic magnetic order [3]: (*i*) an AF phase with two mutually orthogonal antiferromagnets on two sublattices in each *ab* plane and AF order along the *c* axis (ortho-*G*-type phase), (*ii*) a canted-*A*-type AF phase with a non-trivial canting angle between nearest neighbor FM layers along the *c* axis, and (*iii*) a striped-AF phase with anisotropic AF order in the *ab* planes. We elucidate the mechanism responsible for each of these phases by deriving effective spin models which involve second and third neighbor Heisenberg interactions as well as four-site spin interactions going beyond Heisenberg physics, and explain how the entangled spin-orbital superexchange generates spin interactions between more distant spins.

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## Magnetic and electronic properties of $Ce_{11}Ni_4In_9$ and $CeNi_9In_2$

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Polycrystalline $Ce_{11}Ni_4In_9$ compounds and $CeNi_9In_2$ were investigated by means of X-ray diffraction, magnetic, specific heat and X-ray photoelectron spectroscopy (XPS) measurements. $Ce_{11}Ni_4In_9$ crystallize in the orthorhombic $Nd_{11}Pd_4In_9$ –type structure (space group $Cmmm$) with $Ce$ atoms occupying five nonequivalent Wyckoff positions, which $CeNi_9In_2$ crystallize in the $YNi_9In_2$–type structure (space group $P4/mbm$) in which Ce atoms occupying one Wyckoff position. Magnetic measurements indicate that in $Ce_{11}Ni_4In_9$ compound on the Ce atoms has localized magnetic moment which order below $17K$, where in $CeNi_9In_2$ not detected localized moment. Also we report the valence band and the core-level XPS spectra. The results for these last are discussed in the Gunanrsson-Schönhammer model. The values of the coupling energy between $4f$ levels and conduction states $\Delta$ and the number of $4f$ electrons nf are determine. The XPS $Ce3d$ data indicates for both compounds sizable hybridization of the $Ce-4f$ electrons with conduction band. For $CeNi_9In_2$ the $4f^0$ configurations indicate the mixed-valence system. The contribution to the density of states at $E_F$ is found to be dominated by $Ni3d$ states particularly in the case of $CeNi_9In_2$ compound which give the increase of the density states on the Fermi level. The core level $Ni2p_{3/2}$ spectra indicate that in this compound the $Ni3d$ band is incomplete filling.

## Superconductivity in splat-cooled U-T alloys (T=Mo, Pd, Pt)

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Using Mo doping in a combination with splat-cooling technique we are able to stabilize the high-temperature cubic $\gamma$-U structure down to low temperatures. The pure $\gamma$-U structure was obtained in alloys with $\geq$ 13 at.% Mo [1-3]. Those $\gamma$-U materials exhibit a conventional BCS superconductivity with e.g. $T_c \approx 2.1$ K and critical field exceeding 5 T for 15 at.% Mo (UMo15). Mo doping below 11 at.% Mo yields a mixed cubic $\gamma$- and orthorhombic $\alpha$-U phase. In this work we present our study of superconductivity in the UMo6 alloy (with 6 at.% Mo doping). The results are compared with those in UPd5 and UPt5. The XRD patterns of all three samples reveal the existence of the mixed phase. A smooth decrease below 1.5 K and a sharp drop at 0.6 K in the resistivity was observed for UMo6 indicating that $\gamma$-U grains are embedded in the $\alpha$-U matrix, while a single sharp drop was revealed at $T_c \approx 0.8$ K for UPd5 and UPt5. With applying the magnetic fields, the resistivity jumps move to lower temperatures.

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# Tuning of magnetic properties by oxygen content in $(Nd_{1-x}Ca_x)(Ba_{1-y}La_y)Co_2O_{5+\delta}$ layered perovskites ($\delta$ = 0.25 - 0.90)

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The layered perovskites of pure $R\mathrm{BaCo_2O_{5+\delta}}$ ($R$ = lanthanide ion or Y) with cobalt valence equal to 3+ are characterized by the sequence of magnetic and electronic phase transitions observed with increasing temperature: antiferromagnet-ferromagnet (AFM-FM $T_N$=200 - 250 K), ferromagnet-paramagnet ($T_C$=280 - 310 K), and insulator-metal transition ($T_{MIT}$=330 - 360 K), which can be tuned by a substitution at the $R$-, Ba- and Co-sites or by a change of oxygen index $\delta$. We have recently synthesized new compositions of $La^{3+}$ substituted at the $Ba^{2+}$-site up to 10% over a wide range of $\delta$. We have investigated their transport and magnetic properties to develop a phase diagram of $(Nd_{1-x}Ca_x)(Ba_{1-y}La_y)Co_2O_{5+\delta}$ system by comparing properties to previously studied of $Ca^{2+}$ substituted at the $Nd^{3+}$-site system. Combined charge doping by cation substitution and $\delta$ allowed to trace the temperatures of $T_N$, $T_C$ and $T_{MIT}$. For $Nd_{0.9}Ca_{0.1}BaCo_2O_{5.5}$, the AFM-FM transition vanishes and the antiferromagnetic order is absent down to 5 K. For $\delta$ = 0.555 and 0.59, we have found reappearance of AFM-FM transition, accompanied by a decrease of $T_C$. A pronounced drop in the Seebeck coefficient and a significant jump in thermal conductivity are observed near $T_{MIT}$, indicating correlated changes of the electronic and thermal transport. The measurements under pressure performed for $NdBa_{1-y}La_yBaCo_2O_{5+\delta}$ with $y$ = 0 - 0.1 and $\delta$ = 0.5 - 0.55 have revealed pronounced increase of $T_N$. *Work supported by National Science Centre of Poland, contract no. 1662/B/H03/2011/40.*

## 50 years of the Hubbard model: from magnetism to unconventional superconductivity and back

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In my talk I will start with the Hubbard original work on microscopic derivation of the Stoner criterion (1963) on and analysis of the metal-insulator transition (1964). I will allude to the preceding work of Anderson (1959) on the kinetic exchange in Mott insulators. Works in the following two decades concentrated on analysis of phenomena in the regime of correlated electrons, using mainly the Gutzwiller (1963-65) and the Green-function methods. Our introduction of t-J model in 1976 should also be noted in this context. A renewed impetus for the work on the model in the 1980s was caused three factors: (i) introduction of slave-boson approach (1986), (ii) introduction of the concept of real-space pairing by Anderson (1986-8) at the beginning of the high-$T_c$ superconductivity era, and (iii) implementation of the numerical (quantum Monte-Carlo, RG) methods as the test of other methods reliability. Also, the application of the Hubbard model in the last decade to the cold atoms in optical lattices should be noted. Hubbard model is also a point of departure for other models of strong correlated fermions and bosons, e.g., for the Anderson lattice model or the orbitally degenerate Hubbard model, the last particularly in combination with *ab initio* approach.

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## The Boson-Fermion resonant model on a lattice

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Properties of a two-component model of coexisting local electron pairs (hard-core charged bosons) and itinerant fermions coupled via charge exchange mechanism, are reviewed. Firstly, the cases of isotropic and anisotropic pairing of extended $s$ and $d_{x^2-y^2}$ -wave symmetries are analyzed for a 2D square lattice within the mean field and the Kosterlitz-Thouless theories. The superconducting characteristics of this boson-fermion (BF) model are determined as a function of the position of the local pair level and the total particle concentration. Secondly, we present the computation of the superfluid transition temperature from the pseudogap state and phase diagrams of a 3D boson-fermion resonant model within a self-consistent T–matrix approach, which includes pairing fluctuations and bosonic self-energy effect. We analyze salient features of BCS-BEC crossover for various fillings and across the superfluid-insulator transition in the BF model. Our results are discussed in connection with a two-component scenario of preformed pairs and unpaired electrons for high temperature superconductors. We also relate them to resonance superfluidity of ultracold atomic gases in optical lattices.

## Unusual vortex dynamics in magnetic and high-$T_c$ superconductors

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Vortex dynamics in magnetic superconductors might be very unusual due to the interaction between magnetism and superconductivity and reflect the competition between these orders. For high temperature superconductors (HTSC), unusual vortex properties are observed as a result of strong thermal fluctuations present in the superconducting state at temperatures even far from $T_c$. In this review we discuss several intriguing examples of the vortex behavior in magnetic superconductors and HTSC to show the complex nature of the Shubnikov phase in these materials. In particular, the two-step flux penetration process is studied in low-$T_c$ antiferromagnetic superconductors and interpreted as a result of the internal vortex structure with a spin-flop component. For HTSC, the universal character of the Josephson-coupled vortices is shown and analyzed with respect to the melting process of the vortex lattice. Finally, for antiferromagnetic HTSC, we reveal the very well masked interaction between long range magnetic order and superconductivity and show real competition between these effects.

## Interplay of magnetism and superconductivity in Ca and Co-doped $EuFe_2As_2$-based materials

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In this contribution we focus on some physical properties of one of the iron based superconductors family, namely $EuFe_2As_2$-based materials with Ca and Co-doping.

In studied compounds we were able to see multiple phase transitions: starting from paramagnetic (P) state through spin density wave (SDW) ordering to canted antiferromagnetic (C-AF) and finishing in superconducting (SC) state. Even more interesting properties were discovered while magnetic field was applied, i.e. the C-AF state evolves to different C-AF and field induced ferromagnetic (FI-F) phase. Furthermore unique behaviors, such as field induced superconductivity (FI-SC) or disappearing of superconductivity in lower temperatures can be observed.

We suggest that the complex magnetic structure of these compounds is responsible for these remarkable properties. Our opinion is based not only on interpretation of electron transport, ac-susceptibility, heat capacity measurements in wide temperature (2-300 K) and magnetic fields (up to 9 T) ranges; but also on our latest neutron diffraction measurements.

## The magnetic field induced phase separation in the zero-bandwidth limit of the extended Hubbard model with pair hopping

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The phase separation phenomenon involving superconductivity is a very current topic, because it can play a crucial role in determining behaviour in many real compounds and fermions on optical lattices . In our work we have studied a model which is a simple generalization of the standard model of a local pair superconductor with on-site pairing (i. e. the model of hard core bosons on a lattice) to the case of finite pair binding energy. We have analysed the extended Hubbard model with pair hopping in the atomic limit and focused on phase separation and paramagnetic effects of the external magnetic field. The phase diagrams and thermodynamic properties of this model have been determined within the variational approach (VA), which treats the on-site interaction term exactly and the intersite interactions within the mean-field approximation. Our investigation of the general case shows that the system can exhibit not only the homogeneous phases: superconducting (SS) and nonordered (NO), but also the phase separated states (PS: SS-NO). The systems considered exhibit interesting multicritical behaviour including tricritical points. Depending on the values of interaction parameters, the PS state can occur in higher fields than the SS phase (field induced PS). The impact of density-density and magnetic interactions is discussed. Moreover, ground state results beyond VA are also presented.

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# Metallization of atomic solid hydrogen within the extended Hubbard model with renormalized Wannier wave functions

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We have modeled [1] correlated electronic states and the metal-insulator transition by applying the so-called *statistically consistent Gutzwiller approximation* (SGA) and carrying out self-consistent calculations of the renormalized single-particle Wannier functions in the correlated state. The transition to the Mott-Hubbard insulating state at temperature T = 0 is of weak first order even if antiferromagnetism is disregarded. The whole analysis has been carried out for an extended Hubbard model on a simple cubic (SC) lattice and the evolution of physical properties is analyzed as a function of the lattice parameter for the renormalized 1s-type Wannier functions. Quantum critical scaling of the selected physical properties is analyzed as a function of the lattice constant $R \to R_c = 4.1a_0$, where $R_c$ is the critical value for metal-insulator transition and $a_0 = 0.53$ $\AA$ is the Bohr radius. A critical pressure for metallization of solid atomic hydrogen is estimated and is ~ 102 GPa. The behavior of the non-zero temperature critical point in paramagnetic phase is examined.
The work was supported by the Foundation for Polish Science (FNP) under the 'TEAM' program, as well as by the project 'MAESTRO' from National Science Centre (NCN), No. DEC-2012/04/A/ST3/003420.

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## Bound and resonant two-particle states in extended Hubbard model on simple cubic lattice

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Bound and resonant two-particle states within extended Hubbard model on simple cubic lattice in the empty lattice limit are calculated by means of the analytical two-particle $\mathcal{T}$-matrix. The wave functions, dispersion curves along $\Gamma R$ line and the total cross section for two particle scattering within symmetry channels are computed. The actual positions of resonant states within the band and their widths are obtained and compared to approximations known in the literature. The persistence of resonant structures well beyond the regime where the poles of $\mathcal{T}$-matrix exist, are found. The smooth evolution of wave functions with the Hamiltonian parameters between the bound and the band, resonant state limits is shown.

# Posters

## Growth and characterization of $YBa_2Cu_3O_{7-\delta}$ films on $CeO_2$-buffered sapphire

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$YBa_2Cu_3O_{7-\delta}$ (YBCO), in a form of superconducting thin film, is frequently used in passive microwave devices such as superconducting filters or antennas. To avoid high microwave losses in the device it is necessary to grow the YBCO films on the sapphire substrates, with suitable buffer layer to improve matching of the lattice parameters. In this work we study the growth by pulsed laser deposition of YBCO films on the $CeO_2$-buffered R-cut sapphire substrates, with the buffer layer recrystallized prior to the deposition of YBCO. With the help of the atomic force microscopy (AFM) and X-ray diffractometry we determine the optimal thickness and temperature of recrystallization of the buffer layer. We use AFM to examine the dependence of YBCO film roughness on the film thickness, and we study the homogeneity of magnetic flux penetration into the films by magnetooptical imaging. We find that the superconducting critical temperature and the critical current density of the films are very close to similar parameters for the YBCO films grown on lattice-matched single crystalline substrates. It appears that the structural defects in the buffer layer act as very effective vortex pinning centers, resulting in rather high values of the critical current density, suitable for applications.

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## Particle-hole interference of the vibrating quantum impurity coupled to the superconducting lead

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We analyze the energy spectrum and transport properties of a vibrating quantum dot coupled between the superconducting and metallic lead. Proximity effect combined with the electron-phonon interaction induce a series of bosonic modes simultaneously in the particle and hole excitations. Polaronic shift of the quantum dot level can force these particle and hole vibrational states to overlap with each other, leading to their interference. We discuss how such particle-hole interference would manifest itself in the electronic spectrum and in the differential conductance. Furthermore, we examine the role of electron correlations.

## Influence of iron substitutions on the transport properties of $Fe_{1+\delta}Te_{0.65}Se_{0.35}$ single crystals

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We study the ab-plane resistivity and Hall effect in $Fe_{1-y}M_yTe_{0.65}Se_{0.35}$ single crystals, where M = Co or Ni ($0 \le y \le 0.21$). In case of each dopant two types of crystals, with different crystalline quality, are prepared by Bridgman's method using different cooling rates, fast or slow. Both impurities suppress the superconducting transition temperature ($T_c$), but $T_c$ reaches zero at markedly different impurity content: only 3 at.% of Ni, and about 13 at.% of Co; in addition, the suppression is somewhat dependent on the crystal cooling rate. The resistivity at the $T_c$ onset remains almost unaffected by Co doping, while it increases for Ni, with the increase which depends on the crystal cooling rate. The Hall coefficient ($R_H$) is positive for Co doping indicating that hole carriers dominate the transport. For crystals with the Ni content exceeding 6 at.% the $R_H$ changes sign to negative at temperatures between 130 and 180K. We will discuss the correlation between superconducting and normal state properties, and the implications for the understanding of superconductivity in this system.

## Polaron states in a ferromagnetic $CuO_3$ chain

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Historically, the $t$-$J$ model has been recognized as the primary candidate for the description of high-$T_c$ supercoductivity in cuprates. Although exact treatment of the problem has proven to be difficult, a quasiparticle behavior for a single hole was found using the Self Consistent Born Approximation [1]. However, the inclusion of $p$-orbitals, whose importance in charge dynamics of cuprates has long been recognized, causes significant complications in this scheme.

On the other hand, the problem of a single hole moving in a ferromagnetic background is somewhat easier to address, since one can find an exact solution by Green's functions [2] due to a very constrained magnon Hilbert space, while it allows one to gain some valuable insight into the dynamics of a hole coupled to localized spins. Recently, we have solved a 1D model of this kind with two itinerant $p$-bands, and explored the significance of the $p$-$d$ exchange for the system's band structure [3]. Here we examine the effects of the magnon dispersion and find that highly energetic magnons can affect the electronic structure very significantly, even as far as to reduce the number of bands.

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## Stability of bilayer superconductors against thermomagnetic avalanche

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Recently in paper [1] was found increase of stability of the critical state of the superconducting wire with a core and a surface layer of $Nb_3Sn$ and $Nb$, respectively. Stability of critical state of bilayer superconductor has been investigated theoretically in our work. Such composite consist of inner part with critical current $J_2(T)$ $(SCII)$ and thin surface layer thickness $\delta$ with less value of critical current $J_1(T)$ $(SCI)$. On the basis of the general method developed Mints and Rakhmanov [2] in adiabatic approximation ($\tau = 0$) a criterion of stability in order to the magnitude of the external magnetic field was found. The criterion is as follows:

$$B_{1j}(T) = \mu_0 j_1(T)\delta + \\ + B_{02j}(T)\left[1 - \frac{2}{\pi}\arctan\left(\sqrt{\frac{j_1(T)\left|\frac{\partial j_1}{\partial T}\right|}{j_2(T)\left|\frac{\partial j_2}{\partial T}\right|}}\tan\left(\delta\sqrt{\frac{\mu_0 j_1(T)\left|\frac{\partial j_1}{\partial T}\right|}{C(T)}}\right)\right)\right] \quad (1)$$

$B_{02j}(T) = \frac{\pi}{2}\sqrt{\frac{C(T)j_2(T)\mu_0}{\frac{\partial j_2}{\partial T}}}$ – well known criteria of stability for the unmodified superconductors [2]; $C(T)$ - volume specific heat of superconductor, $\delta$ - thickness of the surface layer, $\mu_0 = 4\pi 10^{-7} H/m$, and $T_c$ – critical temperature. For conventional $NbTi$ superconductor with $J_2(0K) = 2\times 10^9 A/m^2$ and $J_1(0K) = 2\times 10^8 A/m^2$ expression (1) give increase field of first flux jump at $4.2K$ more 60%. Thus bilayer superconductor as compared with conventional case has greater stability of critical state. Temperature dependence of $B_{1j}$ and optimal thickness of coat are discussed.

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# Thermal fluctuations in YBCO thin film on MgO substrate

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The $YBa_2Cu_3O_\delta$ thin film was prepared on MgO substrate by PLD method. The thickness of the film is 170 nm and the critical temperature $T_c = 89\,\mathrm{K}$ with $\Delta T = 1.6\,\mathrm{K}$. The critical currents of the film were calculated from the temperature dependencies of the *a.c.* susceptibility using Bean's model. The critical current estimated from the fit parameters is in the order of $10^7\,\mathrm{A/cm^2}$ at 77 K in zero magnetic field. Detailed temperature dependence of resistivity measurements were made in the region from zero resistance up to 300 K. The thermal fluctuations of conductivity were analyzed using Aslamazov – Larkin microscopic approach and the critical exponents were calculated.

# Magnetic phase transitions of FeTe under hydrostatic and biaxial pressure

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FeTe material reveals magnetic phase transition from antiferromagnetic to ferromagnetic order under pressure of about 2 GPa [1]. The tensile strain realized in FeTe thin films induces superconducting state with critical temperature of 13 K [2]. In the work, the influence of hydrostatic and biaxial pressure on crystallographic, magnetic and electronic structure of FeTe compound is investigated from DFT calculations. The results indicate that Te position in the crystal is strongly related with magnetism and superconductivity in iron chalcogenides.

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# The presentation of three-band Eliashberg equations in selected compounds

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In the paper the three-band Eliashberg formalism has been presented. After the dissolution of Eliasberg equation the thermodynamical properties of the superconducting state in one- and multiband systems has been given. In particular in hydrogen, $MgB_2$ and $CaC_6$ observed exceptional properties. Moreover, for oneband systems critical temperature according to McMillan and Allen-Dynes formula has been calculated. In the paper, the example of the numerical results has been presented.

# Electron-phonon pairing mechanism: cuprates with high value of the critical temperature

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The model for the cuprates based on the modified electron-phonon pairing mechanism has been tested. For this purpose, the superconductors with high value of the critical temperature have been taken into consideration. In particular: $YBa_2Cu_3O_{7-y}$, $HgBa_2CuO_{4+y}$, $HgBa_2Cu_{1-x}Zn_xO_{4+y}$, and $HgBa_2Ca_2Cu_3O_{8+y}$. It has been shown that the dependence of the ratio $R_1 \equiv 2\Delta_{tot}^{(0)}/k_BT_C$ on the doping $(p)$ can be properly predicted in the framework of the presented theory; the symbol $\Delta_{tot}^{(0)}$ denotes the energy gap amplitude at the temperature of zero Kelvin, and $T_C$ is the critical temperature. The numerical results have been supplemented by the formula with describes the function $R_1\,(p)$.

# Magnons as pseudo-Goldstones in La-based cuprates: non-linear $\sigma$-model approach

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Pure $La_2CuO_4$ (LCO) is a quantum antiferromagnet with small Dzyaloshinskii-Moriya (DM) and $XY$ anisotropies which break the rotational symmetry of the spin system. The lightly doped compound $La_{2-x}Sr_xCuO_4$ (LSCO) is well described by the anisotropic quantum non-linear $\sigma$-model (QNL$\sigma$M) coupled to the dipole fields representing holes. At $x = x_c \sim 0.02$ the Néel order is destroyed, which is preceded by strong reduction of the magnon gaps. The magnetic anisotropies stabilise the low temperature magnetic phases of LSCO and hence the anisotropy induced magnon gaps are an essential characteristic of the system.

Within the framework of anisotropic QNL$\sigma$M (derivable from microscopic models) we calculate the doping and temperature dependence of the magnon gaps to the one-loop order. Since the rotational symmetry of the spin system is explicitly broken by the small anisotropies, magnons are pseudo-Goldstones. The corrections to the gaps are then required to vanish in the zero bare gap limit. In the previously considered[1] linearised version of QNL$\sigma$M – linear $\sigma$-model (L$\sigma$M), the pseudo-Goldstone behaviour of magnons is a consequence of subtle cancellations of the processes and the spin-dipole coupling takes a complex form. We show that the QNL$\sigma$M is free of these problems. Our results satisfy the pseudo-Goldstone requirement in contrast to the calculations existing in literature. We show that the main effect of hole doping is renormalisation of the spin stiffness and spin-wave velocity. A good agreement with available experimental data is obtained and a new experiment is proposed to further verify the results. The QNL$\sigma$M is shown to agree with the hard constraint limit of the L$\sigma$M.

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# Chemical potential investigations of the surface of ferromagnetic-superconducting multilayers

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Chemical potential $\mu$ is the only one thermodynamical parameter which can be easy measured on low-dimensional systems like thin films or a two-dimensional electron gas. It is especially useful for multilayers because the properties of the topmost layer with thickness about the Debye screening length are investigated.

The method to measure the change of the chemical potential $\Delta\mu = \mu(H) - \mu(0)$ is based on the determination of the change in charge on the measuring capacitor consisting of the sample under investigation and the reference electrode. The idea is closely related to Lord Kelvin's investigations of the contact potential difference. In general, the contact potential difference differs from the chemical potentials difference by the magnitude of the potential difference of the double charged layers present at the surface of bulk metals. If the influence of a magnetic field on the capacitance $C$ and in the work function of the reference electrode is negligibly small then $\Delta Q = -C\Delta\mu/e$, where $e$ is the charge of current carriers.

Measurements of the chemical potential of superconducting and ferromagnetic films in stationary magnetic field were published many years ago [1]. The purpose of the present work is to investigate heterostructures consisting of superconducting and ferromagnetic layers [2]. The heterostructures were characterized by magnetic and transport measurements. Chemical potential investigations were done using the field-modulation technique that significantly increases the sensitivity of the method.

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# Microwave characterization of small high-$T_c$ superconducting thin film filters*

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We report preliminary results of microwave measurements of high-$T_c$ superconducting thin film filters. In the present work we have prepared a number of $YBa_2Cu_3O_{7-x}$ filters for the frequency range of 2.5 GHz on 10 by 10 mm sapphire substrates by pulsed laser deposition. The calculated filter structures were patterned by photolithography, followed by chemical etching. We have measured, by means of a microwave network analyzer, both transmission ($S_{21}$) and reflection ($S_{11}$ and $S_{22}$) coefficients *vs.* frequency, in the temperature range between 60 K and 90 K. Our results are in reasonable agreement with the results of numerical calculations based on circuit theory as well as on electromagnetic field simulations.

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## Alternative equation of motion approach to the single-impurity Anderson model

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Solving the single-impurity Anderson model (SIAM) is the basic problem of the solid state physics. The SIAM model is very important, at present it is also used for systems with quantum impurities, e.g. semiconductor quantum dots and molecular transistors. Its main application is in the scheme of dynamical mean field theory (DMFT) describing the strong correlation electron systems. One method of solving the SIAM problem is the equation of motion (EOM) Green function approach. In this report we present the novel EOM approximation in which we differentiate Green function over both time variables. This differs from commonly used EOM solution by Appelbaum, Penn and Lacroix where the authors take time derivative only over primary time variable. After extending calculations to higher order Green functions we find the new approximate dynamical solution of SIAM. The results are compared with analytical strong and weak coupling limits of SIAM and with the solutions to SIAM problem at intermediate Coulomb repulsion $U$ such as quantum Monte Carlo method and Iterative Perturbation Theory.

# Characterization of the high-pressure superconducting state in the $YH_3$ compound

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In the paper the thermodynamic properties of the high-pressure superconducting state in the $YH_3$ compound have been described ($p$ = 17.7 GPa). By using Eliashberg equations approach the critical temperature and the electron effective mass in wide range of Coulomb pseudopotential have been determined. It has been stated that the value of the critical temperature ($T_C$) decreases from 45.91 K to 27.29 K, if the Coulomb pseudopotential increases ($\mu^\star \in \langle 0.1, 0.3 \rangle$). The dimensionless ratio $2\Delta(0)/k_BT_C$ decreases from 4.38 to 4.20, where the symbol $\Delta(0)$ denotes the value of the order parameter near to the zero temperature. The ratio of electron effective mass to the band electron mass is high, and its reaches maximum equal to 2.42 for the critical temperature.

# Perturbation of the $^{57}Fe$ quadrupole interaction at superconducting transition in $Ba_{0.6}K_{0.4}Fe_2As_2$

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Optimally doped '122' compound $Ba_{0.6}K_{0.4}Fe_2As_2$ has been studied by $^{57}Fe$ Mössbauer spectroscopy in the temperature range 4.2 – $300K$ with the particular attention paid to the superconducting transition region around $37K$. Spectra do not contain magnetic components. Hence, the spin density wave (SDW) is completely destroyed by doping in contrast to the parent compound $BaFe_2As_2$ [1]. Spectra are composed of two symmetrical quadrupole doublets. Doublet with narrow lines and smaller splitting contributes about 95% to the absorption cross-section and originates from the iron in the sites unperturbed by dopant. The second doublet is characterized by rather broad lines and has larger splitting. It is due to iron perturbed by dopant. The quadrupole interactions drop at the transition to the superconducting state on both iron sites and recover upon further cooling. This effect could be explained by development of the Cooper pairs, and subsequent raise of the carrier density on the Fermi surface leading to the effective shielding of the electric field gradient (EFG). Widening of the superconducting gap with falling temperature separates bosonic carriers from the remainder of the system and causes recovery of the EFG.

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# Variational and Diffusion Quantum Monte Carlo calculation of magnetization and spin gaps in small graphene quantum dots

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We investigate electron correlation effects in graphene nanoflakes using variational and diffusion quantum Monte Carlo (QMC) techniques. Since its exfoliation by Geim and Novoselov in 2004, graphene attracts the attention of the scientific community, due to their unique physical properties and promising potential for technological applications. Recent works using configuration-interaction method have shown that in graphene quantum dots correlations can play an important role resulting e.g. in the spin depolarization effect after adding one extra electron to the charge neutral system. In this work, Variational Monte Carlo technique is applied to optimize the trial many-body wave function, formed from Hartree-Fock orbitals multiplied by a Jastrow factor. The optimized solution is used as a starting point for Diffusion Monte Carlo method. Using these methods, the ground state energies, magnetization and energy spin gaps for small graphene flakes are determined. The results are analyzed as a function of a dielectric constant strength.

# Anderson-Kondo lattice Hamiltonian from modified Schrieffer-Wolff transformation: Exchange interactions

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We apply canonical perturbation expansion for the periodic Anderson model in direct space to derive the so-called Anderson-Kondo lattice model. The transformation is accomplished by treating as a perturbation only the part of the hybridization term connected with high energy processes (involving the largest in the system intraatomic Coulomb interaction between $f$ electrons) and replacing it with the virtual processes in higher orders. As a result, we obtain the effective Kondo ($f$-$c$) and super exchange ($f$-$f$) interactions. The calculations are carried out up to the fourth order of expansion, taking into account both the two- and the three-site processes. In this manner, the effective Hamiltonian can be used to analyze the magnetic or the paired states, as well their coexistence in heavy-fermion systems. At the end, we present hybridization matrix elements for cerium compounds in tetragonal symmetry.

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# Phase separation near half-filling point in superconducting compounds

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We present the model of superconducting ceramics using single band extended Hubbard Hamiltonian. We investigate the simultaneous presence of antiferromagnetism (AF) and the d-wave superconductivity (SC) in the coherent potential (CP) approximation applied to the on-site Coulomb repulsion $U$. We consider the hopping interaction, $\Delta t$, the inter-site charge-charge interaction, $V$, (capable of creating SC), and the single site Hund's type exchange interaction, $F_{\text{in}}$, (capable of creating AF). The influence of these interactions on the separation of superconducting and antiferromagnetic phases near the half-filling point is investigated. Impact of initial bandwidth of unperturbed DOS on both phases is also considered. Results are compared with the experimental data for YBaCuO and NdCeCuO compounds.

## Penetration of magnetic field in a single crystal of $MgB_2$: Meissner holes and flux avalanches

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Flux distributions were imaged and analyzed during remagnetization of a $MgB_2$ plate ($860 \times 660 \times 400 \mu m^3$) using the magneto-optical technique. This technique yields pictures of field penetration and provides measurements of the normal component of induction on the sample surface. A crystal of $MgB_2$ was grown from solution at the pressure of 15 kbar and the temperature of $1800C^\circ$. The features of magnetic induction patterns at the boundary between oppositely magnetized parts in the $MgB_2$ crystals were studied. It was found that near the edge of the crystal in magnetic field, the opposite field magnetization was present and a Meissner hole [1] was observed (the area where the annihilation of neighboring vortex and antivortex occurred and the cavity-free flux appeared). The distribution of the magnetic induction in the range of Meissner-hole generation was calculated. We studied avalanche structures of the magnetic flux as a result of thermomagnetic processes in a bulk sample. Here, the magnetic flux avalanche structure turns out to be similar to a "fingerprint", unlike films which are characterized by dendritic structures. Induction profile of finger-like structures in the longitudinal and transverse cross section has a convex shape. Other peculiarities (quasi-static and dynamical ones) of the magnetic field penetration were considered.

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# Electronic structure of Kondo lattice systems; nonmagnetic $Ce_2CoSi_3$ and antiferromagnetic $Ce_2RhSi_3$

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$Ce_2CoSi_3$ has a Kondo temperature of $T_K$ ~50 K [1] while $Ce_2RhSi_3$ is antiferromagnetic below $T_N$ = 4.5 K with estimated $T_K$ ~ 9 K [2]. Therefore, these isostructural compounds should be located in different places of the Doniach phase diagram. In order to explore the electronic structure of both systems, their valence bands have been studied by photoemission spectroscopy for a series of photon energies between 88 eV and 140 eV. A Ce 4d-4f resonance is observed near 120 eV, where a contribution from Ce 4f electrons is enhanced. The 4f spectral functions determined experimentally show Kondo peak at the Fermi energy and its spin-orbit partner at 275 meV. The differences in the electronic structure between the compared compounds are discussed on a basis of the photoemission results and full-potential local-orbital (FPLO) calculations with LSDA+U approach.

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# Jack polynomials as model wave functions of fractional quantum Hall effect

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Fractional quantum Hall effect (FQHE) is remarkable behavior of quasi-two-dimensional electrons in high magnetic field, depending primarily on the Landau level filling factor $\nu$ (dimensionless ratio of electron and magnetic flux densities). It turned out to be hard to find explicit form of the wave functions describing FQHE, so various approximate methods were developed. Jack polynomials turned out to be the convenient family of symmetric polynomials describing many-electron states in FQHE. In this work we present the ideas needed to introduce Jack polynomials (1-4), such as the partition of a natural number, the ring of symmetric polynomials, and the basic structure of this space (important basis, inner product). After defining Jack polynomials we present well-known wave functions containing symmetric polynomials, such as the $\nu = 1/3$ Laughlin and the $\nu = 5/2$ "Pfaffian" state, and propose new wave functions, and compare them with non-explicit wave functions derived from computations.

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# Size of Cooper pairs dependence on orbital parameters in a two-orbital superconductor

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We study the sizes of Cooper pairs in the negative $U$ Hubbard model depending on band filling as well as inter- and intra- orbital interactions. The size of Cooper pairs $\xi_{pair}$ is estimated from the a wave function of the Cooper pairs $\psi(\mathbf{r})$:

$$\xi_{pair} = \sqrt{\frac{\int \mathrm{d}\mathbf{r}|\psi(\mathbf{r})|^2\mathbf{r}^2}{\int \mathrm{d}\mathbf{r}|\psi(\mathbf{r})|^2}}.$$

The calculations are limited to a two-orbital model. In particular, we show substantial dependence of temperature in the particular sets of model parameters. Finally, we compare the obtained results of the sizes of Cooper pairs to the corresponding penetration depths [1].

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# Coexistence of ferromagnetism and superconductivity in bilayer heterostructures

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Ferromagnet / superconductor heterostructures are an attractive model system for studying the proximity effect and interaction between magnetism and superconductivity. In this work we present recent experimental results on heterostructures composed of ferromagnetic $La_{0.67}\ Sr_{0.33}\ MnO_3$(LSMO) and superconducting $YBa_2\ Cu_3\ O_7$ (YBCO) bilayers grown by dc sputtering method. We have investigated the transport and magnetic properties of the set of samples in a wide temperature range from 2 to 400 K and in fields up to 14 T. We have observed the co-existence of ferromagnetism and superconductivity in these heterostructures and the influence of a magnetic LSMO layer on superconducting properties of an adjacent YBCO layer. The Nernst effect has been studied revealing the correlation of some characteristic points on the temperature dependence of the Nernst signal with the upper critical field.

# Resistive and magnetoresistive properties of composite materials based on carbon nanotubes

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Carbon nanotubes (CNT) are an important new class of technological materials that have numerous novel and useful properties. There are many applications of it in perspective. So, knowledge in the selection of physical properties must be priority target for researches. In our investigation we studied the resistive and magnetoresistive properties, which are very important for practical using. Moreover, an influence of impurities on these resistive properties was also investigated. The models of conductivity which can adequately describe behavior of the electrical transport in the wide temperature range and magnetic fields up to 6T, are considered. Fitting results for three conductivity models (activation, tunneling and hopping) are presented and shortly discussed.

# XPS study of superconductiong $LiTi_2O_4$ and $LiTi_{2-x}Cu_xO_4$ sol-gel derived powders and thin films

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In this work XPS studies of structure of lithium titanate and copper doped lithium titanate are presented. Both, powder and thin films samples, were prepared by sol-gel method. Lithium acetate, butoxytitanium and ethanol were used as the reagents. Additionally copper nitrate was added as a Cu dopant source for preparation of $LiTi_{2-x}Cu_xO_4$. Thin films were deposited on a quartz glass substrates by a spin coating technique at a rate of 120 rps. Both, powder and thin films samples were calcinated in argon atmosphere at various temperature in a range from 500 $^o$C to 600 $^o$C for 20 hours.

The crystal structure of prepared samples were investigated by X-ray diffraction (XRD), while the oxidadation states of the elements were examined by X-ray photoelectron spectroscopy (XPS) method. XRD measurements confirmed spinel phase of all investigated samples. It is well known that superconductive properties of lithium titanate are strongly correlated with structure and oxidation state of Ti ions. According to comparision literature data with lattice parameter, (that was calculated on the basis of Bragg's formula), we selected samples, that gives hope to obtain superconductive material. XPS investigations revealed mixture of $Ti^{3+}$ and $Ti^{4+}$ ions. Dependence between calcination temperature as well as amount of Cu dopant and $Ti^{3+}$ - $Ti^{4+}$ proportion was observed.

# Phase diagram of two dimensianal extended Hubbard model with intersite magnetic interactions, a Monte Carlo study

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Extended Hubbard model with intersite magnetic interactions is analyzed by means of grand canonical Monte Carlo simulations on two dimensional square lattice. Simulations were performed using two differents paths (with either chemical potential or temperature constant) to get accurate results for range of electron concentration $n \in < 0, 1 >$ and temperature. Additionaly extensive histogram analysis was performed to determine precise location of tri-critical point. Binder cumulant ratio technique was used to obtain data for infinite lattice. Such analysis unveiled full phase diagram of the model in which three phases are present: (anti)ferromagnetic, non-ordered and phase separation as well as corresponding phase transitions of either first or second order.

# Crystal field states in superconducting $CeFeAsO_{1-x}F_x$ ($T_{sc}$ = 41 K)

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There is going on a debate about the existence and the role played by the crystal field (CEF) in compounds containing 3d/4f/5f atoms/ions both in ionic and intermetallic compounds. We, i. e. the magnetic community, has been successful to find well-defined crystal-field states in superconducting $CeFeAsO_{1-x}F_x$ ($T_{sc}$ of 41 K for $x$ =0.16) at 18.7 and 57 meV originating from the $Ce^{3+}$ ions.

We have derived CEF parameters of the relevant symmetry of the $Ce^{3+}$ site and we have calculated the single-ion properties of the $Ce^{3+}$ ions. We discuss their contribution to properties of the whole compound.

The magnetism of the maternal non-superconducting CeFeAsO compound will be discussed owing to its quite high Neel temperature of 140 K and the influence of the antiferromagnetic order within the Fe sublattice on the Ce states.

The electronic structure for other isostructural rare-earth oxypnictides will be derived and compare to experimental literature data.

presented by D. M. Nalecz

# Magnetoconductance of the Corbino disk in graphene bilayer in biased graphene bilayer

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Quantum transport through an impurity-free Corbino disk in graphene bilayer pierced by the magnetic flux $\Phi_D$ is investigated by means of mode-matching analysis for the Dirac equation. In analogy to the Corbino disk in a monolayer studied in Ref. [1], periodic conductance oscillations (with the mean value corresponding to the universal quantum conductivity [2]), are present at pseudodiffusive regions of the field-doping parameter plane. At the Dirac point, the oscillations magnitude now depends not only on the radii ratio $R_\mathrm{o}/R_\mathrm{i}$, but also on the interlayer hopping integral $t_\perp$, whereas the period $\Phi_0 = 2(h/e)\,\ln(R_\mathrm{o}/R_\mathrm{i})$ remains the same as in the monolayer. Also, we find that for the system parameters satisfying the condition $R_\mathrm{o}/R_\mathrm{i} \simeq [\hbar v_F R_\mathrm{i}/(2t_\perp)]^{4/k}$ (with $k$ the odd integer) the conductance oscillations vanish for either normal Corbino or the Andreev-Corbino setup. A detailed comparison with the behavior of Schrödinger fermions in the two-dimensional electron gas (2DEG) is provided. In particular, we show that the disk in graphene bilayer with strong bias potential between the layers reproduces the transport characteristics of the disk in a monolayer rather than those of the disk in 2DEG.

The work was supported by the Foundation for Polish Science (FNP) under the 'TEAM' program.

[1] A.Rycerz, *Magnetoconductance of the Corbino disk in graphene*, Phys. Rev. B **81**, 121404(R) (2010) pp. 1–4.

[2] G. Rut and A. Rycerz, *Pseudodiffusive conductance, quantum-limited shot noise, and Landau-level hierarchy in biased graphene bilayer*, arXiv:1307.7093 (unpublished).

## Pseudodiffusive charge transport and Landau-level hierarchy in biased graphene bilayer

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We discuss, by means of mode-matching analysis for the Dirac equation, how splittings of the Landau-level (LL) degeneracies associated with spin, valley, and layer degrees of freedom affect the ballistic conductance of graphene bilayer [1]. The results show that for wide samples ($W \gg L$) the Landauer-Büttiker conductance reaches the maximum $G \simeq se^2/(\pi h) \times W/L$ at the resonance via each LL, with the prefactor varying from $s = 8$ if all three degeneracies are preserved, to $s = 1$ if all the degeneracies are split. In the absence of bias between the layers, the degeneracies associated with spin and layer degrees of freedom may be split by manipulating the doping and magnetic field; the conductance at the zeroth LL is twice as large, while the conductance at any other LL equals to the corresponding conductance of graphene monolayer. The presence of bias potential allows one also to split the valley degeneracy. The charge transfer at each LL has pseudodiffusive character, with the second and third cumulant quantified by $\mathcal{F} = 1/3$ and $\mathcal{R} = 1/15$ (respectively). In case the electrochemical potential is allowed to slowly fluctuate in a finite vicinity of LL, the resulting charge-transfer characteristics are still quantum-limited, with $\mathcal{F} \simeq 0.7$ and $\mathcal{R} \simeq 0.5$ in the limit of large fluctuations. The above values of $\mathcal{F}$ and $\mathcal{R}$ are also predicted to be approached in the limit of high source-drain voltage difference applied.

[1] G. Rut and A. Rycerz, arXiv:1307.7093 (unpublished).

# Mechanical studies of NbN-$SiO_2$ sol-gel derived films

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In this work the studies of mechanical properties of $NbN - SiO_2$ films are reported. To obtain these films, sol - gel derived $Nb_2O_5 - SiO_2$ coatings were nitrided at 1200 ℃. As it was presented previously, such prepared films exhibit superconducting properties. However superconductivity depends on $NbN/SiO_2$ ratio and the thickness of the film. Nanoindentation results show that the samples consist of the regions of the different nanohardness. These areas can be assigned to NbN grains and to surrounding amorphous silica matrix. Existence of these two different phases influences both mechanical properties and superconducting properties of the samples.

## One–dimensional array of double–well potentials: cluster–perturbation theory for the Hubbard models for fermions and fermion-boson mixtures

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One-dimensional fermion and boson-fermion Hubbard models are studied by means of the cluster perturbation theory. The system is composed of weakly coupled dimers. The energy spectrum and eigenstates of separate dimers are calculated analytically for the fermionic model and numerically for the boson-fermion model. Then, the perturbation expansion with respect to the interdimer hopping integral is applied in order to determine the ground state properties of the entire system. Such an array of double-well potentials can be created by superimposing two optical lattice potentials differing in period by a factor of two [1].

[1] S. Fölling, S. Trotzky, P. Cheinet, M. Feld, R. Saers, A. Widera, T. Müller and I. Bloch, Nature **448**, 1029 (2007)

# Proximitized NbN/NiCu and NbTiN/NiCu Superconductor/Ferromagnet Nano-bilayers for single proton detection

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Superconducting single-photon detectors (SSPDs) based on resistive hotspot formation in a superconducting nanostripe upon optical photon absorption are presently regarded as the best high-performance, ultrafast photon counters, especially in the optical telecommunication range. The current devices are typically ~ 4–$nm$–thick and ~ 100–$nm$–wide, either $NbN$ o $NbTiN$, stripes formed into a large area meander (e.g., $10 \times 10\mu m^2$) and operating at the temperature much lower than the superconductor critical temperature $T_C$. Their main performance limitations come directly from their geometry; namely, quantum efficiency is limited by the actual thickness of the stripe (light absorption in a metallic film), while the counting speed is restricted by the very large kinetic inductance of a superconducting meander. One of the possible approaches towards the SSPD performance improvement is modification of a superconducting material. In our case, we implement superconductor/ferromagnet ($S/F$) nano-bilayers consisting on $nm$–thick $NbN/NiCu$ and $NbTiN/NiCu$ films. At the detector operating temperature, the $S/F$ bilayers are fully proximitized, however, utilization of a few–$nm$–thick $F$ cap layer on top of the $S$ film allows to enhance the device critical current due to an extra pinning mechanism and, simultaneously, reduces the value of the kinetic inductance of the meander by means of the proximity effect and increased quasiparticle recombination rate at the interface. In addition, the increased total thickness of the S/F stripe, as compared the pure $S$ one, results in its increased optical absorption, what translates into higher detection efficiency. We have fabricated a variety of $NbN/NiCu$ and $NbTiN/NiCu$ bilayers, performing dc magnetron sputtering at very high substrate temperatures. After the $NbN$ (or $NbTiN$) deposition, the films were, subsequently inserted into a $NiCu$–dedicated system, where the NbN (or NbTiN) surfaces were first pre-cleaned using ion-beam etching at a rate of about $0.2nm/s$, and then coated with $Ni_{0.52}Cu_{0.48}$ overlayers. The individual thicknesses of the $S$ and $F$ films varied from 3 to $10nm$. We selected a $Ni_{0.52}Cu_{0.48}$ alloy an $F$ layer, since it is reported to have the Curie temperature on the order of $20K$, well above $T_C$ our $S$ layers. In our presentation, we discuss structural properties of our $S/F$ bilayers with the main emphasis on the epitaxy of the individual films and the quality of the $S-F$ interface (TEM cross-sections with the atomic-level resolution). Electron transport of patterned bilayers, such as resistance and critical current density dependences on temperature, and current-voltage characteristics, were studied and compared to those of uncovered $S$ layers.

## Magnetic domain-controlled phase diagram and vortex pinning in the superconductor-ferromagnet bilayers

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In this study we evaluate the influence of the geometry of magnetic domain pattern on the superconducting transition temperature ($T_c$) and the vortex pinning in superconductor(SC)/ferromagnet(FM) bilayers. In the bilayers the SC layer is niobium, and the FM layers are built from Co/Pd multilayers with perpendicular magnetic anisotropy. After predefining the magnetic domain pattern at $T > T_c$ we extract the dimensions of domains from AFM images. Next, we measure the magnetoresistance in the superconducting state in perpendicular magnetic field $H$, from which we obtain the $T_c(H)$ dependence, and, from the Arrhenius plots of the resistance, the activation energy for vortex pinning $U(H)$. We find that both $T_c(H)$, and $U(H)$ strongly depend on the magnetic domain width $w$. In particular, at large $w$ the $T_c(H)$ shows two maxima at $H \neq 0$. The decrease of $w$ leads to the enhancement of vortex pinning, while large $w$ enhances flux flow along domains. These features are somewhat similar to those observed by us previously in the case of FM layers built from Co/Pt, but different values of $w$ lead to some differences between the two systems.

In addition, we will also show the comparative results for bilayers built from oxide films, which were grown using a pulsed laser deposition method, with $SrRuO_3$ as the FM layer, and $YBa_2Cu_3O_7$ as the SC layer.

# Influence of lithium doping on the thermodynamic properties of graphene based superconductors

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It has been recently observed that the conventional electron-phonon mediated superconducting phase in graphene can be induced by doping its surface with the lithium adatoms [G. Profeta *et al.*, Nature Phys. **8** (2012) 131]. Due to the emerging interest in this field we present our theoretical discussion on the thermodynamic properties of such novel graphene structures within the strong-coupling Eliashberg formalism. We show, that together with the increase of the adatom doping, from one ($LiC_6$) to two ($Li_2C_6$) lithium atoms per unit cell, the critical temperature ($T_C$) changes from 8.55 K to 21.83 K. Such trend is also observed for other thermodynamic properties which moreover differ from the predictions of the Bardeen-Cooper-Schrieffer theory. In particular, the zero-temperature energy gap to the critical temperature ratio: $R_{\Delta}^{LiC_6}$=3.72 and $R_{\Delta}^{Li_2C_6}$=4.21; the ratio of the specific heat for superconducting and the normal state: $R_{C}^{LiC_6}$=1.47 and $R_{C}^{Li_2C_6}$=1.79; and the parameter connected with the zero-temperature thermodynamic critical field: $R_{H}^{LiC_6}$=0.167 and $R_{H}^{Li_2C_6}$=0.144. Finally the electron effective mass at $T_c$ is calculated to be: $(1.62m_e)_{LiC_6}$ and $(2.48m_e)_{Li_2C_6}$.

## Electronic band structure and photoemission states of $Bi_{1.96}Mg_{0.04}Se_3$

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We present theoretical band structure calculations and ultraviolet electron photoemission spectroscopy (UPS) of a topological insulator $Bi_{1.96}Mg_{0.04}Se_3$. Our calculations were based on the first-principles density functional theory with general gradient approximation using Wien 2K package [1]. The spin-orbit interaction was including by a second-variation method. The (166 ITC) crystal structure taken from [2] was optimized. In consequence, 4% decrease of volume and and 3% decrease of ratio c/a was made. This modified structure was multiplied three times in a and b direction in order to place proper amount of Mg in the lattice. Final crystal structure P3m1 with 135 atoms was used for the calculations. As a result metallic band structure was obtained with conduction band extended from -5.6 eV up to 0.16 eV. It composes mostly from Se p states. Comparison of total DOS with ultraviolet photoemission spectrum shows similar features.

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# Anomalous magnetic, thermodynamic and transport properties of ruthenium perovskites $Ca_{1-x}Sr_xRuO_3$

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The ruthenium perovskite $SrRuO_3$ is a metallic ferromagnet with the Curie temperature of $T_C \simeq 163$ K. In the $Ca_{1-x}Sr_xRuO_3$ system, dilution of the strontium sublattice by calcium atoms with smaller atomic radii leads to decrease of the Curie temperature and to decrease of the ruthenium magnetic moments. The ferromagnetic order disappears at a critical concentration of strontium $x_{cr} \simeq 0.27$, which means that at this concentration takes place the quantum phase transition between the itinerant ferromagnet and a metallic paramagnet. All materials with $x < x_{cr}$ demonstrate metallic conductivity and do not show the magnetic order down to the temperature of 0.4 K.

In this report, investigations of the magnetic, thermodynamic and transport properties of the samples with the strontium concentration $x$ varying from 0 to 0.4 are presented and discussed. The ferromagnetic compound $Ca_{0.6}Sr_{0.4}RuO_3$ ($T \simeq 20$ K) shows typical Landau-Fermi-liquid behaviour with $C/T$ = const and $\rho \sim T^2$. All the materials with $x < x_{cr}$ show anomalous properties. The magnetic susceptibility in the range of temperatures from approx. 10 to 100 K behaves as $\chi \sim T^{1-\lambda}$ with concentration dependent value of $\lambda$ parameter. The heat capacity and the electrical resistivity demonstrate transitions from the Fermi-liquid at very low temperatures to the anomalous behaviour with $C/T \sim \log T$ and $\rho \sim T^{3/2}$ at higher temperatures. The Fermi-liquid behaviour is restored in the external magnetic field.

# Fermi surfaces of heavy-fermion $Ce_2Ni_3Ge_5$, $CeNiGe_3$, and exotic $YNiGe_3$ superconductors

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Electronic structures of pressure-induced $Ce_2Ni_3Ge_5$ [1], $CeNiGe_3$ and multiband BCS-like $YNiGe_3$ [2] superconductors have been calculated by the full potential local-orbital (FPLO) code [3], employing both the local density approximation (LDA) and LDA+U approaches. Our computed Fermi surfaces (FSs) of the two investigated Ce-based heavy-fermion superconductors reveal specific nesting properties. They support a presence of antiferromagnetic spin fluctuations (SF) as a glue of unconventional superconductivity in these systems. Meanwhile, the topology of the FS in $YNiGe_3$ enables multiband superconductivity, which can explain the observed anomalous jump at the superconducting critical temperature in its specific heat.

**References:** [1] M.J. Winiarski, M. Samsel-Czekała, J. Alloys Compd. 560, 123 (2013). [2] M.J. Winiarski, M. Samsel-Czekała, Solid State Commun. (2013). [3] FPLO9.00-34; www.FPLO.de.

# Synthesis, electrical properties and single crystal growth of a novel $Sr_5Pb_3ZnO_{12}$ oxide

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Polycrystalline samples of a novel $Sr_5Pb_3ZnO_{12}$ (531-Zn) oxide were synthesized by a solid-state reaction method. Crystallographic structure of the compound was studied by powder x-ray diffraction (XRD) together with Rietveld refinement method. 531-Zn exhibit hexagonal lattice (space group *P-62m*, no. 189) with infinite chains of edge-sharing $PbO_6$-$ZnO_6$ polyhedra surrounded by $Sr^{2+}$ ions. Electrical properties of the compound was studied on polycrystalline samples by means of impedance spectroscopy. Material was found to be a dielectric with low DC conductivity. Several-hundred-micrometer-long needle-like single crystals were successfully grown from polycrystalline powder using flux method employing NaCl as the flux. Obtained crystals were characterized by means of confocal microscopy and scanning electron microscopy (SEM).

## Enhancement of the critical temperature induced by the quantum size effect in superconducting nanofilms

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In the recently fabricated high quality superconducting nanofilms the interplay of quantum confinement and pairing correlations has a significant influence on the superconducting parameters. It is caused by the fact that in the quasi-two-dimensional superconducting nanofilms quantization of the transverse electron motion leads to the increase of the density of states each time when the bottom of the transverse sub-band passes through the Fermi level. In the present paper, we have numerically investigated the Bogoliubov-de Gennes equations for superconducting Al nanofilm and found that for the appropriate thickness, for which the subsequent sub-bands passes through the Fermi level, the critical temperature and the order parameter abruptly increase up to several times in comparison with the bulk value. Our results explain the oscillations of the critical temperature observed experimentally for the superconducting nanofilms [1, 2].

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## Diagrammatic Expansion of Gutzwiller Wave Function

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A systematic diagrammatic expansion for Gutzwiller-wave function (DE-GWF) is presented. The method is numerically very efficient and allows for a detailed analysis of the phase diagram. As a result, we construct phase diagram for the Hubbard model comprising superconducting and paramagnetic states. We also provide comparison of the nodal Fermi velocity with experimental data for high-temperature superconductors as well as with other theoretical method. The applicability of the method to the case of periodic Anderson model will be also briefly discussed.

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# Penetration depth of bulk $Tl_2Ba_2Ca_2Cu_3O_y$ and $Tl_{0.58}Pb_{0.4}Sr_{1.6}Ba_{0.4}Ca_2Cu_3O_y$ superconductors

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The penetration depths of bulk $Tl_2Ba_2Ca_2Cu_3O_y$ and $Tl_{0.58}Pb_{0.4}Sr_{1.6}Ba_{0.4}Ca_2Cu_3O_y$ superconductors with the critical temperatures $112K$ and $114K$, respectively, were determined from the *a.c.* susceptibility measurements. When the samples are in the Meissner state, the dispersive components of ac susceptibility as well as their temperature dependences reflect the changes of the penetration depths at various temperatures. In these bulk ceramic superconductors the penetration depths are the order of few micrometers and they are comparable to the grain size in the ceramics.

## Critical currents of YBCO 1:2:3 films on silver substrates

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The $YBa_2Cu_3O_\delta$ films were obtained directly on silver substrates by the sedimentation processes. The thickness of these films is in the order of hundred micrometers. The temperature dependencies of the *a.c.* susceptibility of the films were measured and analyzed. The critical temperatures of these specimens were obtained from the dispersion part of *a.c.* susceptibility and they vary from 90 K to 93 K. The critical currents were calculated from the absorption part of *a.c.* susceptibility using Bean's model. The temperature dependencies of the critical currents were fitted using the Ginzburg–Landau strong coupling limit approach.

## Continuous unitary transformation approach to the strongly correlated systems

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Theoretical methods for studying the correlation effects can be broadly classified in three main categories: perturbative expansions, exact analytical solutions and numerical methods. These approaches have their specific advantages and shortcomings. Many-body systems, where strong electron correlations play an essential role, have been however difficult to study because such methods often turned out to be insufficient. In this presentation we discuss an alternative theoretical tool based on the selfadapted continuous unitary transformation. This procedure has been introduced by F.Wegner and independently by K.Wilson. Its algorithm belongs to the renormalization group techniques allowing to investigate the correlation effects beyond a perturbative framework.

On a technical level the method develops unconventional scaling in the entire Hilbert space, gradually disentangling the low from high energy modes. Continuous diagonalization of the relevant Hamiltonian is achieved via the set of scaling (flow) equations. We shall give a few examples how this continuous unitary transformation technique can be applied to strongly correlated systems in the symmetry broken states, for instance: superconductors (where gauge symmetry is broken), ferromagnets (where rotational symmetry is broken) and the Kondo impurities hybridized with external charge reservoirs.

# Hall effect of ultrathin niobium in the Si/Nb/Si trilayers

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One of the fundamental problems in nanoscience research is a question on the nature of the ground state in confined systems, particularly in the case of the superconducting (SC) materials. It is well established that the reduction of the thickness of SC films leads to the superconductor-insulator transition (SIT). The usual assumption is that the SIT is induced by disorder which reduces mean-free path. In this work we demonstrate an example of the SIT the origin of which may be more complex. We study the structural and magnetotransport properties in a series of Si/Nb/Si trilayers grown by magnetron sputtering at room temperature. The thickness of Nb, $d$, is varied from 20 nm down to 1.1 nm with a fixed Si thickness of 10 nm. The high-resolution TEM and the X-ray diffraction indicate that for $d > 6$ nm the films are polycrystalline, while they become amorphous for smaller $d$. The Hall effect measurements reveal that the positive Hall coefficient, characteristic for bulk Nb, starts decreasing for $d$ below 6 nm, and eventually changes sign into negative for $d$ below 2 nm. The slight nonlinearity of the Hall voltage versus magnetic field is observed in the thinnest samples ($d$ about 1.3 nm), what may indicate the presence of two types of carriers. The possible origins of this effect include the modification of the niobium band structure, or the contribution of the Nb-Si interface to the conduction. We will also show that the SIT in this system involves a transition from the SC to the metallic non-SC phase.

# Band filling effects on coherence lengths and penetration depth in the two-orbital d-wave Hubbard model of superconductivity

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The two-orbital superconducting state is modeled by inter-site intraorbital Hubbard correlations together with inter-orbital pair-transfer interactions. The critical temperature is mainly governed by intraorbital attractive interactions and it can pass through an additional maximum as a function of band filling. For the certain number of electrons the clear interband proximity effect is observable in the superconducting state of the band with a smaller gap. The influence of band fillings and orbital site energies on the temperature dependencies of two-component superconductivity coherence lengths and magnetic field penetration depth is analyzed. The presence of proximity effect is probably reflected in the relative temperature behaviour of characteristic lengths. The present investigations are continuation of the previous studies on s-wave superconductors [1,2].

[1] G Litak, T Örd, K Rägo, A Vargunin, Physica C 483 (2012) 30–33.
[2] G Litak, T Örd, K Rägo, A Vargunin, Acta Physica Polonica A 121 (2012) 247–251.

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