Book of Abstracts

From Spins to Cooper Pairs and Back: 2nd International Conference on Magnetism and Superconductivity in Selected Systems

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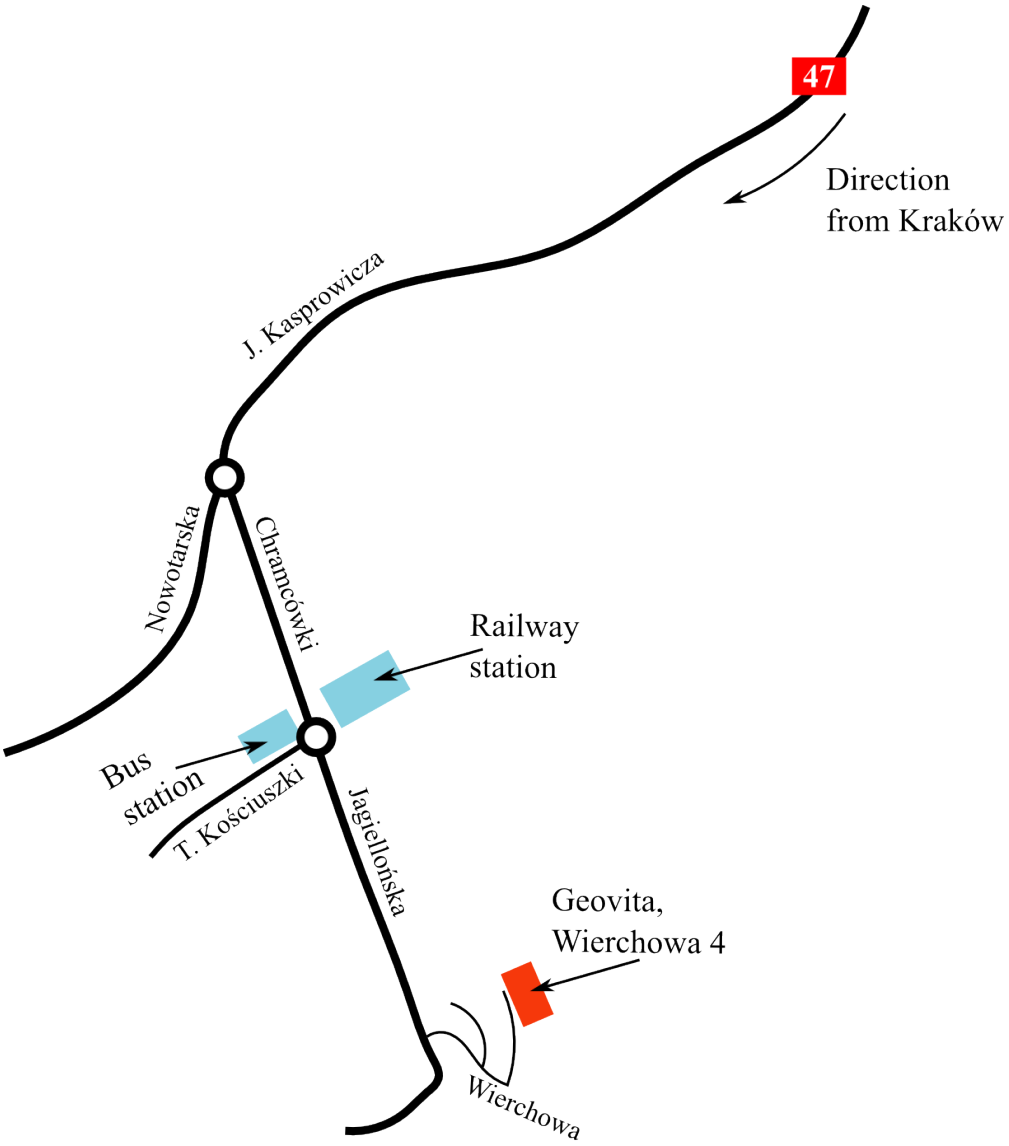

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Superconductivity at $T_c = 2mK$ in the quantum critical heavy-fermion antiferromagnet $YbRh_2Si_2$ due to competing nuclear order

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Unconventional superconductivity often occurs in the vicinity of quantum critical points (QCPs) in antiferromagnetic (AF) heavy-fermion metals. However, no superconductivity has so far been observed near some of the canonical heavy-fermion QCPs, such as the one induced by a magnetic field in $YbRh_2Si_2$, raising the question about the generality of this paradigm. Here, we will explore the possibility of reaching the quantum critical regime by sufficiently weakening the AF order through its coupling to nuclear spins at very low temperatures, instead of applying a pair-breaking magnetic field. To this end, we discuss results of magnetic and calorimetric measurements on $YbRh_2Si_2$ down to $T = 1\,\mathrm{mK}$. They reveal the onset of a hybrid nuclear-electronic type of AF order dominated by the Yb-derived nuclear spins at T_A slightly above 2 mK and the subsequent development of superconductivity at $T_c = 2\,\mathrm{mK}$. The initial slope of the upper critical field curve, $B_{c2}(T)$, at T_c is found to be as large as - $B'_{c2} \cong 25\mathrm{T/K}$. This indicates that the effective charge-carrier mass must be of the order of several $100\,m_\mathrm{el}$, implying that the superconducting state is associated with the Yb-derived $4f$ electrons. The apparent heavy-fermion superconductivity in $YbRh_2Si_2$ may be called "high T_c", in the sense that it is limited by an exceedingly high ordering temperature of nuclear spins ($T_\mathrm{A} \gtrsim 2mK$ as compared to common values in the nK range). Also, we briefly address the theoretical possibility of superheavy-fermion superconductivity based upon an underlying nuclear Kondo effect. In conclusion, we ascribe the formation of Cooper pairs in $YbRh_2Si_2$ to the critical fluctuations associated with the unconventional QCP of this antiferromagnet, which are revealed when the primary electronic order is diminished by the competing nuclear order. Our results demonstrate a new means to reach an AF QCP and provide further evidence that superconductivity in the vicinity of such an instability is a general phenomenon.

Charge order in Cuprates

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In the last few years charge density waves (CDWs) have been ubiquitously observed in cuprates (see e.g. ref. 1) and are now the most investigated among the competing orders in the high-temperature superconducting cuprates.

A wealth of new experimental data raise fundamental issues. In this communication (2), based on the occurrence of dynamically fluctuating CDWs within a frustrated phase separation mechanism (3), we reproduce the complex experimental temperature vs. doping phase diagram. We also rationalize the recent Hall effect measurements (4) in high magnetic field, which indicate a Fermi-surface reconstruction in $YBa_2Cu_3O_y$ for doping $p < 0.16$ at low temperature and a rapid variation of the number of carriers from small pockets to a large Fermi surface between $p_c \approx 0.16$ and $p^* \approx 0.19$.

The last doping is where the pseudogap crossover temperature $T(p)$ extrapolates to zero. In our theory T is related to the mean-field CDW instability line i.e. T^* is interpreted in terms of a reduction of the density of states due to incipient CDW. Strong fluctuations reduce the mean-field critical line to a much lower bona fide dome-shaped CDW transition line $T_{CDW}(p)$, ending at $T = 0$ into two CDW-QCPs, at $p'_c \approx 0.08$ and $p_c \approx 0.16$. The whole region between T^* and T_{CDW} is characterized by increasingly stronger fluctuations and for doping $p_c < p < p$, the rapid change of the interaction mediated by CDW-fluctuations allows us to fit the measured rapid Hall number variation. Furthermore in the region of phase diagram between T^* and T_{CDW} we obtain different onset lines $T_{onset}(p)$ for dynamical CDW order. These various lines are obtained by limiting the reduction effect of fluctuations on the mean-field line with different infrared frequency cut-offs. In our theoretical scheme the various infrared cut-offs are representative of the time scales of the probes (x-ray scattering, NMR,âĂę) by which the different onset lines are detected.

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2. S. Caprara, C. Di Castro, G. Seibold, and M. Grilli, arXiv:1604.07852v1
3. C. Castellani, C. Di Castro, and M. Grilli, Phys. Rev. Lett. 75, 4650 (1995); S. Andergassen et al.Phys. Rev. Lett. 87, 056401 (2001).
4. S. Badoux et al. Nature 531, 210 (2016)

Charge density wave order and the carrier density in cuprate superconductors

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Pseudogap is a partial gap that opens in the normal state of the cuprate superconductors. Its origin and connection to Mott insulator at low doping p remains ambiguous and its relation to the charge-density wave (CDW) order, that reconstructs the Fermi surface at intermediate p, is still unclear. I will discuss the CDW order and its connection to the electronic transport properties of these materials. Furthermore, I will present the Hall coefficient measurements in magnetic fields up to 88 T, which revealed that the Fermi-surface reconstruction by the charge order in YBCO ends sharply at a critical doping $p = 0.16$, distinctly lower than the pseudogap critical point at $p^* = 0.19$. This shows that pseudogap and charge order are separate phenomena. We find that the change of carrier density from $n = 1 + p$ at high p to $n = p$ at low p starts at p^*. This sharp loss of 1.0 carrier per Cu atom is a new signature of the pseudogap. I will discuss some possible underlying mechanisms.

Metamorphoses of electronic structure of FeSe-based superconductors

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The electronic structure of FeSe, the simplest iron based superconductor, conceals a potential of dramatic increase of T_c that realizes under pressure or in a single layer film. This is also the system where nematicity, the phenomenon of a keen current interest, is most easy to study since it is not accompanied by the antiferromagnetic transition like in all other Fe-SC's. Here we overview recent ARPES data on electronic structure of FeSe-based superconductors: isovalently substituted crystals, intercalates, and single layer films, trying to clarify its topology and possible relation of this topology to superconductivity, finally focusing on temperature evolution of the band structure. We show that the band structure evolution with lowering temperature is in line with increase of correlations and can be understood as a screening of near neighbor hopping due to aniferromagnetic spin or orbital fluctuations. The later seems more reasonable, considering these fluctuations as a precursor of nematic transition.

Extended t-J model: Quantative comparison with experiment

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We review briefly the universal properties of high-Tc superconducting systems, as well as present their very recent understanding within the combined concepts of strong correlations and real-space pairing. The considerations are based on effective one-band model, in which the strong (but finite) direct Coulomb interactions (the Hubbard- and intersite-terms) are explicitly included, in addition to the standard structure of the t-J model. The parameters of this extended model are estimated on the basis of the three-band p-d model of CuO_2 plane. The solution is of the full-Gutzwiller-wave-function type, in which the renormalized mean field theory (RMFT) represents the zeroth-order solution within the diagrammatic approach developed in real space. The main motivation is to compare our principal results to available experimental data in a quantitative manner. Those include: (i) doping independence of the Fermi velocity in the nodal direction; (ii) kinetic-energy gain in the superconducting state (non-BCS feature); (iii) value of optimal doping and that of disappearance of superconducting phase, and (iv) doping dependence of the Fermi wave vector and of the effective mass, both determined in the nodal direction. We believe that our approach provides probably the first such a comprehensive discussion of selected basic experimental properties of high-Tc superconducting systems.

The work was supported by the National Science Centre (NCN) through the Grant MAESTRO, No. DEC-2012/04/A/ST3/003420. The cooperation with Dr. Jan Kaczmarczyk on the early stage of this project is appreciated. The discussions with Profs. Dirk van der Marel from Unversite de Geneve and Adam Kaminski from Iowa State Univ. have been enlightening.

Defects, Disorder, and Strong Electron Correlations in Orbital Degenerate, Doped Mott Insulators

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We elucidate the effects of defect disorder and *e*-*e* interaction on the spectral density of the defect states emerging in the Mott-Hubbard gap of doped transition-metal oxides, such as $Y_{1-x}Ca_xVO_3$. A soft gap of kinetic origin develops in the defect band and survives defect disorder for *e*-*e* interaction strengths comparable to the defect potential and hopping integral values above a doping dependent threshold; otherwise only a pseudogap persists. These two regimes naturally emerge in the statistical distribution of gaps among different defect realizations, which turns out to be of Weibull type. Its shape parameter k determines the exponent of the power-law dependence of the density of states $(k-1)$ and hence distinguishes between the soft gap regime $(k \geq 2)$ and the pseudogap one $(k < 2)$. Both k and the effective gap scale with the hopping integral and the *e*-*e* interaction in a wide doping range. The motion of doped holes is confined by the closest defect potential and the overall spin-orbital structure. Such a generic behavior leads to complex non-hydrogen-like defect states that tend to preserve the underlying C-type spin and G-type orbital order and can be detected and analyzed via scanning tunneling microscopy.

High-temperature superconductivity in hydrogen-rich materials and cuprates

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Theoretical calculations and experiments have found that T_C of sulfur hydride (H_3S) can be as high as 203 K at pressure close to 150 GPa [1,2]. Motivated by the recent progress in this area, we have carried out calculations to explore in detail the thermodynamic properties of superconducting H_3S. The very large values of electron-phonon coupling strength $\lambda = 2.067$ [3], caused that our investigations were conducted within the framework of the strong-coupling Eliashberg theory (with and without lowest-order vertex corrections), which allows us to describe the thermodynamic properties of sulfur hydride with an experimental accuracy [4,5].

Simultaneously, we focus our attention on the development of the theoretical model, which can be use to describe the properties of d-wave superconducting state in cuprates. Containing the electron-phonon and electron-electron-phonon pairing mechanism, we can reproduced with a very high accuracy the measurement results obtained for the hole-doped superconductors [6].

1. A. Drozdov, M. I. Eremets, I. A. Troyan, *et al.*, Nature **525**, 73 (2015).
2. I. Troyan, A. Gavriliuk A, R. Ruffer, *et al.*, Science **351**, 1303 (2016).
3. R. Akashi, M. Kawamura, *et al.*, Phys. Rev. B **91**, 224513 (2015).
4. A.P. Durajski, R. Szczęśniak, L. Pietronero, Ann. Phys. **528**, 358 (2016).
5. A.P. Durajski, R. Szczęśniak, Y. Li, Physica C **515**, 1 (2015).
6. R. Szczęśniak, A.P. Durajski, Supercond. Sci. Technol. **27**, 125004 (2014).

Skutterudite-related $Ce_3M_4Sn_{13}$ and $La_3M_4Sn_{13}$ (M=Co, Ru, Rh); A pathway from f- and d-electron correlations to superconductivity

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The skutterudite-related $Ce_3M_4Sn_{13}$ (M = Co, Ru, Rh) heavy fermions exhibit a behavior characteristic of the Ce-based systems with comparable Kondo and magnetic energy scales, and can be near a magnetic quantum critical point (QCP). In the critical regime, even weak perturbations, e.g., disorder can cause significant effects by changing the nature of the quantum macro state. Therefore, investigations of atomic scale disorder in the form of defects and vacancies, granularity, and the effective increase in disorder by doping have received renewed attention because of novel phenomena in these strongly correlated materials. The main goal of this review is to compare the low-temperature properties of selected $Ce_3M_4Sn_{13}$ and $La_3M_4Sn_{13}$ compounds. We discuss a nanoscale inhomogeneity as a bulk property of $La_3M_4Sn_{13}$ and $Ca_3Rh_4Sn_{13}$, leading to *high-temperature* inhomogeneous superconducting state with the critical temperature $T_c^\star$, higher than T_c of the bulk phase. The pressure coefficients $dT_c^\star/dP$ for the inhomogeneous phase, almost twice large as those of Tc, are discussed according to the Eliashberg theory. Our data suggest a larger lattice stiffening in the *high-temperature* phase. We argue that the pressure effect enhanced by disorder strongly determines the magnitude of T_c and dT_c/dP. We also suggest that in the case of inhomogeneous superconductivity, the pressure dependence of the density of states at the Fermi level is more pronounced than in the bulk superconductor, and also may contribute to larger value of $T_c^\star$ and $dT_c^\star/dP$.

Exchange-bias effect in complex perovskite oxides

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A brief review of exchange bias (EB) effect in managanites, cobaltites and ruthenates with perovskite structure will be presented. In general, the most relevant common feature of these compounds, leading to an appearance of EB effect is an intrinsic phase separation. Parameters of EB effect may be very effectively tuned by even tiny change in chemical composition and moderate external hydrostatic pressure due to their impact on AFM/FM phases ratio. The EB effect may be also induced by the Dzyaloshinsky-Moriya interaction across the interface between FM clusters and surrounding AFM matrix. As particular examples will be discussed:

- phase-separated $CaMn_{0.9}Ru_{0.1}O_3$ manganite, exhibiting strong enhancement of EB effect under pressure,

- $CaMn_{0.9}Nb_{0.1}O_3$ - for this compound EB effect may be induced by the Dzyaloshinsky-Moriya interaction across the interface between FM clusters and surrounding G-type AFM phase.

- $La_{0.9}Ba_{0.1}CoO_3$ cobaltite, exhibiting at low temperatures the FM cluster-glass behavior and pressure dependent EB effect.

- Mn-doped $SrRu_{1x}Mn_xO_3$ perovskite ($0.2x0.3$), here EB effect originates from exchange interactions at the interface of nanoscale FM clusters coexisting with dominant AFM phase at the boundary of the first-order FM/AFM transition.

Charge-density-wave state induced by structural distortion in heavy-fermion compounds $Ce_3M_4Sn_{13}$ (M=Co, Ru, Rh)

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In previous reports a structural transition from a cubic phase of $Yb_3Rh_4Sn_{13}$ - type to the super lattice variant has been reported at $\sim$ 160 K for a series of skutterudite-related $Ce_3M_4Sn_{13}$ compounds, where M=Co, Ru or Rh. We have simulated the low-temperature XRD diffraction patterns of the distorted unit cell using written for that purpose DISTorX program. The method proposed here for x-ray diffraction analysis obtains the XRD patterns from the atomic positions and allows to investigate crystal structure without imposed symmetry operations. We have indicated crystallographic plane where distortion occurs and explained possible origin of CDW in these materials. We have also shown that distortion caused by the charge density wave leads to a very small shift in peak position, and a significant change in the intensity of diffraction lines.

Looking for new unconventional superconductors among (Y;Th)T_2M_2 systems (where T = transition metal and M = Si, Ge)

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The discovery of exotic superconductivity in YFe_2Ge_2 by Zou et al. (2014) motivated us to undertake comprehensive investigations of the formation, band structure and physical properties of Th-, Y-, La-, Sc- and Lu-based 1:2:2 silicides and germanides. We present the crystal and calculated electronic structures of several (Y;Th)T_2M_2 compounds (T = d-electron transition metal, and M = Si or Ge) as well as their low-temperature physical properties. Most representatives of the series crystallize in the tetragonal $ThCr_2Si_2$-type structure (space group $I4/mmm$), while only very few of them adopt the tetragonal $CaBe_2Ge_2$-type structure (space group $P4/nmm$). Significantly, superconductivity in these ternaries is restricted mainly (but not only) to those with the primitive crystallographic unit cells which force an occurrence of numerous quasi-two-dimensional Fermi surface sheets allowing for multi-band superconductivity.

Unconventional superconductivity of the noncentrosymmetric $LaNiC_2$ and the effect of presure

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Superconductivity in the noncentrosymmetric $LaNiC_2$, and its evolution with pressure, is analyzed basing on the *ab initio* computations and the full Eliashberg formalism. Calculations of the electronic structure and the electron-phonon coupling are reported in the pressure range 0-15 GPa. The thermodynamic properties of the superconducting state are determined numerically solving the Eliashberg equations. We found that already at $p = 0$ GPa, the superconducting parameters deviate from the BCS-type, and a large value of the Coulomb pseudopotential $\mu^\star = 0.22$ is required to get the critical temperature $T_c = 2.8$ K consistent with experiment. If such $\mu^\star$ is used, the Eliashberg formalism reproduces also the experimentally observed values of the superconducting order parameter, the electronic specific heat jump at the critical temperature, and the change of the London penetration depth with temperature. This shows, that the triplet pairing or multiple gaps are not necessary to explain deviation of the above-mentioned parameters from the BCS ones. Under the external pressure, calculations predict continuous increase of the electron-phonon coupling constant in the whole pressure range 0-15 GPa, consistent with the experimentally observed increase in T_c for the pressure range 0-3 GPa, but inconsistent with the drop of T_c above 4 GPa and the disappearance of the superconductivity above 7 GPa, reported experimentally. This supports the hypothesis of the formation of a new high-pressure electronic phase, which competes with the superconductivity.

The Fulde–Ferrell–Larkin–Ovchinnikov phase in iron-based superconductors

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In a standard theory of the superconductivity one uses an idea of the Cooper pairs. In the BCS theory, these pairs have zero total momentum. However, it turns out that under some conditions the Cooper pairs can have non-zero total momentum. This phase, called Fulde–Ferrell–Larkin–Ovchinnikov phase, can be realized in low temperatures and high magnetic fields. One expects a realization of this phase in organic or heavy fermions superconductors. Some experimental and theoretical works suggest also a possibility of the realization of this phase in iron-based superconductors (see A. Ptok, J. Phys.: Condens. Matter **27**, 482001 (2015) and reference therein).

Iron selenite (FeSe) is the simplest representative of the iron-based superconductors. The absence of a magnetic order makes it a good candidate to test many physical properties such as the pairing mechanism. The possibility of the existence of unconventional phase in high polarised regime has been reported experimentally (S. Kasahara, *et al.* Proc. Natl. Acad. Sci. USA **111**, 16309 (2014)). Here, without determination of the mechanism of superconductivity, we show a method for studying the superconducting properties using a combination of the density functional theory (DFT) and the Cooper pair susceptibility calculation. It is shown that this compound has a tendency to stabilise the FFLO phase. This is confirmed for other gap symmetries which suggests that this phase is generic.

Insight into a hybridization of Ce 4f electrons with photoemission spectroscopy

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We studied selected cerium intermetallics by means of photoemission spectroscopy. The investigated systems were: magnetic Kondo lattice (Ce_2RhSi_3), Kondo lattice ($Ce_2Co_{0.8}Si_{3.2}$) and a mixed valence compound ($CeNi_9In_2$). Angle integrated photoemission spectra consist of peaks related to f^0, ${f_{7/2}}^1$ and ${f_{5/2}}^1$ final states and the last one is often called a Kondo resonance. The ${f_{5/2}}^1$ peak carries information about hybridization between conduction band and f-electrons: V_{cf}. It has a high intensity for $Ce_2Co_{0.8}Si_{3.2}$, lower for Ce_2RhSi_3 and in the case of mixed valent $CeNi_9In_2$ it is visible only in 4f related spectral weight and much broadened. Angle resolved photoemission spectroscopy (ARPES) revealed that the intensity of ${f_{5/2}}^1$ peak varies along a Fermi surface what may be a fingerprint of the anisotropic V_{cf} [1].

We acknowledge collaboration on photoemission spectroscopy studies with the following people: H. Schwab, F. Forster, I. Vobornik, F. Reinert. Ł. Walczak, B. Penc, J. Adell. The synthesis of $CeNi_9In_2$ was made by Yu. Tyvanchuk and Ya. M. Kalychak.

[1] P. Ghaemi et al., *Phys. Rev. B* **77**, 245108 (2008).

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What is important for High Temperature Superconductivity; multiple experiments with CLBLCO

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The $(Ca_xLa_{1-x})(Ba_{1.75-x}La_{0.25+x})Cu_3O_y$(CLBLCO) cuprate superconductor has a unique phase diagram (see Fig. 1) allowing one to test which of the normal state phenomenon is correlated with superconductivity. This is because the variable x changes only the $Cu-O-Cu$ buckling angle and bond distance. These quantities determine the overlap integrals between Cu orbitals, and hence, the hopping t or super-exchange J parameters. Other parameters such as disorder, symmetry, or valance are x independent. The doping is set solely by the oxygen content y. The parameter x also impacts the superconducting properties, and in particular Tc. Therefore, CLBLCO allows us to look for correlations between electronic properties and superconducting properties with x as an implicit parameter. I will present measurements of: t using angle resolved photoemission spectroscopie (ARPES), J at underdoped CLBLO using muons and Raman scatteing, and at optimal doing using resonance inelastic x-ray scatteign (RIXS), measurements of pseudogap temperature T^* using NMR, and, finally, preliminary data of the charge density wave (CDW) critical temperature T_{cdw} using resonance elastic x-ray scatteign (REXS). We find that T_c is correlated with J, and is independent of T_{cdw} or T^*. This suggests that CDW and the pseudogap phenonema are matterial properties irelevent for superconductivity, while orbital overlaps manifested as super-exchange are an important ingredient in the superconducting glue.

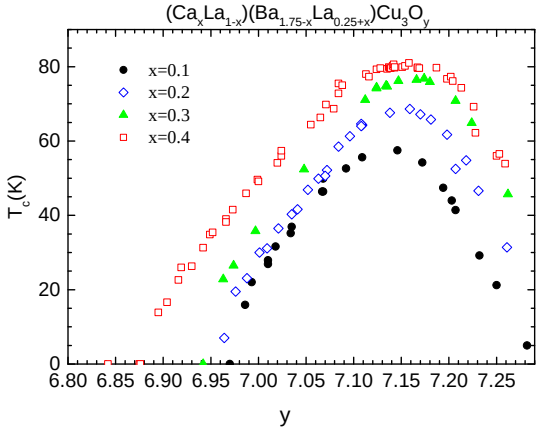

Figure 1: The CLBLCO phase diagram showing the Neel temperature T_N, the glass temperature T_g and the superconducting critical temperature T for four different families (different x) as a function of doping (y).

Strange metals, fermion signs and entanglement.

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The strange metals as observed in high Tc superconductors and other correlated electron systems are arguably the greatest enigma of condensed matter physics. The difficulties are rooted in the fundamentals of physics: the lack of a general mathematical mathematical framework to deal with strongly interacting fermions at finite density, the fermion sign problem. The holographic duality as discovered in string theory is the first method yielding a precise description of non-Fermi liquids. These holographic strange metals are suggestively similar to the laboratory variety, at the same defeating the basic principles of bosonic field theory. These are quantum critical phases with scaling properties alien to those computable with conventional methods. Remarkably their entanglement entropies demonstrate that their ground states are more densely entangled than deemed possible. I will present some first indications that this is rooted in the sign structure. Using the so-called nodal surface (zeroÕs of the wavefunction) as a measure, this fermionic entanglement structure can be addressed in a geometrical language. The nodal surface of a Fermi liquid is characterised by a scale but using a particular Ansatz a quantum critical state can be described characterised by a fractal nodal surface and an entanglement entropy bearing similarity to those of the holographic strange metals.

From Cooper Pairs to entangled spins: single quantum dot three terminal devices

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Three terminal devices with quantum dots connected to three normal or two normal and a superconducting electrode have been studied [1-3]. We are interested in their use as efficient heat to energy converters and/or spin current sources. The usefulness of the device as energy harvester is characterized by the Seebeck coefficient and thermoelectric figure of merit or the power factor. The energy flow from the hot electrode together with energy filtering provided by quantum dots leads to a voltage bias between the cold electrodes [1]. The presence of the superconducting electrode (case 2) allows to study the interplay between the crossed Andreev reflections and direct electron tunneling between two normal electrodes. This case is contrasted with the experimental data [4] on a similar planar structures. If external magnetic field is applied the three terminal hybrid system is a source of pure spin current which can be electrically controlled. *(The work has been performed in collaboration with B.R. Bułka, T. Domański,U. Eckern, G. Michałek, and B. Szukiewicz , and partially supported by the the National Science Centre âĂŞ Poland- grant DEC-2014/13/B/ST3/04451)*

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Superconducting-ferromagnetic heterostructures

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Recent years have brought rapid development of the studies of thin-film based superconducting-ferromagnetic structures. Ferromagnetism and superconductivity are two long-range orders, which are mutually exclusive in the bulk. However, in thin-film-based heterostructures these two long-range orders interact, leading to a wealth of unique phenomena, which broaden the understanding of physics involved, and create potential for applications in spintronics. In this talk, I will review some of the experiments performed recently in this field, focusing mainly on two topics. One of them is the proximity effect at the ferromagnet-superconductor interface, leading to the generation and manipulation of the spin triplet supercurrents. The other is the magnetic-domains-control of the phase diagram and vortex dynamics in superconducting films.

Effect of Co and Ni doping on the electronic structure of $FeTe_{0.65}Se_{0.35}$

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It is known that Co or Ni doping suppresses superconductivity in $FeTe_{0.65}Se_{0.35}$ and changes the Hall coefficient from positive to negative at low temperatures [1]. The transport data indicate that the influence of Co can be understood as simple electron doping, whereas the effect of Ni is more complex. In order to clarify these effects, we studied undoped $FeTe_{0.65}Se_{0.35}$ and both Co and Ni doped systems by means of angle resolved photoemission spectroscopy (ARPES) and X-ray photoemission spectroscopy (XPS). Clear band shifts related to filling with electrons are observed for the doped systems. However, in the case of Ni the transfer of electrons to valence band is less efficient. It is also found that doping removes one or two of three hole pockets for Co and Ni doped compounds. The third hole pocket, which was seen in the data for undoped $FeTe_{0.65}Se_{0.35}$ but has not been resolved for the doped samples, has the largest volume and probably is not removed with doping. XPS data show that electron doping shifts the Fe 2p level towards lower binding energies.

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Acknowledgements: Transport properties of the crystals were characterized by V. L. Bezusyy and M. Z. Cieplak.

Perturbation theory of phase transitions in quantum dot attached to two superconducting leads

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A theoretical study of a single-level quantum dot with local Coulomb repulsion attached to two generally different superconducting leads at zero temperature will be presented. We use the Nambu formalism and the standard many-body diagrammatic representation of the impurity Green functions to formulate the Matsubara perturbation expansion in the interaction strength up to the second order. This simple method yields excellent results for the position of the singlet-doublet impurity quantum phase transition boundary as well as for the single-particle quantities in the singlet phase. This is confirmed by comparing with the numerical renormalization group (NRG) method results. We used the perturbation expansion to interpret the existing experimental data on the phase boundary. The very satisfactory outcome suggests, that heavy numerical tools such as NRG and/or quantum Monte Carlo are not necessary in a class of generic situations and can be safely replaced by a perturbative approach.

Dot-ring nanostructure: Rigorous analysis of many-electron effects

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We discuss the quantum dot-ring nanostructure (DRN) as canonical example of a nanosystem, for which the interelectronic interactions can be evaluated exactly. The system has been selected due to its tunability, i.e., its electron wave functions can be modified much easier than in, e.g., quantum dots. We determine many-particle states for $N_e = 2$ and 3 electrons and calculate the 3- and 4-state interaction parameters, and discuss their importance. For that purpose, we combine the first- and second-quantization schemes and hence are able to single out the component single-particle contributions to the resultant many-particle state. The method provides both the ground- and the first-excited-state energies, as the exact diagonalization of the many-particle Hamiltonian is carried out. DRN provides one of the few examples for which one can determine theoretically all interaction microscopic parameters to a high accuracy. Thus the evolution of the single-particle vs. many-particle contributions to each state and its energy can be determined and tested with the increasing system size. In this manner, we contribute to the wave-function engineering with the interactions included for those few-electron systems.

The work was supported by the National Science Centre (NCN) through the Grant MAESTRO, No. DEC-2012/04/A/ST3/003420.

Metallization of molecular and atomic hydrogen in 2D under high pressure

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Using our original method - the **E**xact **D**iagonalization **ab I**nitio approach (EDABI), we discuss, on the microscopic level, the process of metallization of the hydrogenic systems. We provide the model of concomitant atomization and metallization of the two-dimensional, square molecular lattice, with semilong-range interactions, with the metallization pressure $p_M = 0.166Ry/a_0^2$. We analyze also a two-dimensional, triangular atomic plane with very long-range interactions, appearing under high pressures in diphosphine at $p = 150GPa$ (cf. N. Degtyarenko, E. Mazur arXiv:1603.00405). We show that, under sufficiently high pressure, the system undergoes a metallization-like transition.

The work was supported by the project MAESTRO from Nat. Sci. Centre (NCN), Grant No. DEC-2012/04/A/ST3/00342.

High temperature superconductivity in the t-J-U model: influence of interlayer coupling and formation of charge ordered phase

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The Gutzwiller wave function solution of the t-J-U model is considered by using the diagrammatic expansion method. In the first part of the talk the superconducting phase is analyzed for the case of the bilayer crystal structure. The chosen pairing symmetry is a mixture of the $d_{x^2-y^2}$ symmetry within the layer and the so-called $s^{\pm}$ symmetry for the interlayer contribution. The analyzed interlayer terms correspond to the interlayer electron hopping, the interlayer exchange coupling, and the interlayer pair hopping. For the sake of completeness, some results for the case of the bilayer Hubbard model are also provided.

In the second part of the talk the role of the intersite Coulomb repulsion (proportional to V) in the formation of the charge ordered phase (CDW) is analyzed within the modyfied Gutzwiller approximation (SGA). In particular, we show that the the stability of the CDW phase appears only above a critical value of V and in the limited doping range, δ. At the same time, the effect of the intersite repulsion on the paired phase is negative (it decreases the upper critical doping for the superconductivity disappearance). The antiferromagnetic phase is not significantly influenced by sizable V.

The work was supported by the National Science Centre (NCN) through the Grant MAESTRO, No. DEC-2012/04/A/ST3/003420.

How to deal with hard problems: Examples from graph theory

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Many fundamental graph problems (such as coloring, vertex cover, dominating set, Hamiltonicity) are hard and there is little hope to find polynomial-time algorithms solving them. On the other hand, such problems are of practical importance.

We can look for algorithms which are "less exponential" than previous algorithms in order to extend maximum size problems which can be practically solved. A second approach is to find approximation algorithms which are guaranteed to yield solution close to optimal (edge coloring, vertex cover). A third approach is to restrict the domain of the problem (planar graphs, chordal graphs). Fast algorithms can be created for graphs that are recursively constructed (trees, Halin graphs). Algorithms typically employ a dynamic programming technique.

Our aim is to show examples for the second and the third case. Graph algorithms are expressed by means of the Python language package *graphtheory*.

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Electron-phonon and electron-electron interactions in two-band fermion systems

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Two effective polaronic Hamiltonians are derived from Hamiltonians being some extensions of periodic Anderson model. These extensions consist in the incorporation of Holstein and Hubbard terms representing interactions of a local fermion (electron, hole) with local phonons and with the other fermion, respectively. The first case includes a potential standing for the hybridization assisted by local phonons which can lead to the nonmagnetic Kondo effect. Additionally, a pair-exchange potential emerges due to the making use of a Lang-Firsov type transformation. A simplified case is investigated. Different properties of the ground state and the critical temperature are found. The second case takes into account the possibility of interaction of a local electron (hole) pair with total spin equal zero with phonons in each of the bands. It is shown that this can bring about the appearance of three- and four-fermion terms in the transformed Hamiltonian. Next, the ground state and some other properties of simplified cases are examined.

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Interplay of topology and magnetism: gap and spin texture engineering of topological surface states

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Topological insulators (TI) represent a new quantum phase of matter defined by a bulk insulator with Z_2-invariant topology that guarantees the existence of topologically protected helical surface states (TSS). The presence of an exchange field, which violates time reversal invariance reveals novel spin related phenomena derived from the peculiar coupling of topology and magnetism. We discuss the realization of magnetically induced novel quantized states, such as the quantum anomalous Hall phase and the topological magnetoelectric effect, in the three-dimensional Bi_2Se_3 topological insulator. Based on *ab-inito* calculations, we investigate the behaviour of the Dirac TSS of Bi_2Se_3 at the interface with an atom-thin Cr film and show, that the metallic or gapped character of the TSS can be controlled by the Cr film. As the thickness of the magnetic film increases stepwise from one to three atomic layers there is a double Dirac-metal to gapped transition. Moreover, correlated with the gap evolution, a modification of the TSS spin texture, which undergoes a double circular skyrmion to circular meron transition, takes place. We analyze the origin of the transitions and prove that the thickness of the Cr film provides a simple, accessible and effective mechanism to control and alter the topological states of Bi_2Se_3. These results open a route to the realization of the exotic topological magnetoelectric effect and to the manipulation of the TSS required for the development of TI-based spintronic.

Topological Crystalline Insulators - from protected surface states to Quantum Spin Hall Effect

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Topological crystalline insulators (TCI) are materials that have nontrivial band structure topology protected by point-group symmetries. It has been discovered that (Pb,Sn)Te and (Pb,Sn)Se solid solutions host metallic Dirac helical surface states protected by mirror symmetry of the rock-salt (RS) structure and are perfect objects for studying phase transition between normal narrow-gap semiconductor and TCI. During the talk I will discuss the properties of surface electrons in the IV-VI TCIs. In particular, it has been shown that the energy spectra and the spin textures of the surface states strongly depend on the surface orientation. For example, in contrast to the surface states observed on the (100) surface, the Dirac cones at (111) surface are well separated and no interacting. I will describe ARPES and spin-resolved ARPES experiments performed on the bulk as well as on thin $Pb_{1-x}Sn_xSe$ layer, which confirm the theoretical predictions. Finally, I will also discuss how the reduced dimensionality in TCIs thin layers affects the surface states and hence their topological properties. Using a tight-binding approach we demonstrate that in (111)-oriented thin films of SnSe and SnTe the energy gaps depend in an oscillatory fashion on the layer thickness. The calculated topological invariant indexes and edge state spin polarizations show that in the negative energy gaps regions (20-40 monolayers) a 2D topological insulator phase appears. In this range of thicknesses edge states are obtained with Dirac cones having opposite spin polarization in their two branches and the quantum spin Hall effect (QSHE) is predicted to exist.

Strongly Correlated Networks of Transition Metal and Oxygen

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Transition metal (M) oxides forming 3-dim and 2-dim corner-shared networks build of the MO_6 octahedra with nearly 180 deg M-O-M bonds exhibit some of the most spectacular physical properties known, which are derived from strong correlations among charge, spin and orbital degrees of freedom of the 3d electrons. I will review some of these characteristics in perovskites AMO_{3d} starting from the ferroelectric M=Ti (d^0), through multiferroic M=Mn (d^4), enhanced thermoelectric M=Co (d^6 and d^7) and finishing with the layered superconducting M=Cu (d^9). I will use a simple description of these materials based on the crystal field theory, which allows development of the essential parameters describing properties and establishing design rules for predicting new properties and designing new compounds. While semi-ÂŋâĂŘempirical design rules are not 100 % accurate, they have a virtue of simplicity and can be intuitively comprehended. The unique properties of perovskites arise from their unusual chemical versatility and structural intricacy, which can be tailored through selection of specific A-site cations, their fractions, ionic sizes and valences, spin states, and electronic orbital orderings, as well as the content and vacancy ordering of oxygen. Taking into account all these parameters in crystal field theory is relatively easy, while it is practically not possible in a more rigorous theory. The success of crystal field theory in describing properties of the d^0 - d^8 perovskites indicates that it should be also possible to use it for understanding superconducting d^9 cuprates.

Piezomagnetic switching and persistent magnetoelastic memory in uranium dioxide

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Uranium dioxide is, by far, the most thoroughly studied actinide material as it is a key component in nuclear energy applications. Its magnetoelastic properties, however, remain an unsolved puzzle resulting from strong couplings between magnetism and lattice vibrations. UO_2 is a Mott-Hubbard insulator with well-localized $5f$-electrons and its magnetic state is characterized by a non-collinear antiferromagnetic structure and multidomain Jahn-Teller distortions. In this talk I will show that single crystals of UO_2, subjected to magnetic fields up to 95 T in the magnetic state, exhibit the abrupt appearance of positive linear magnetostriction leading to a trigonal distortion. Upon reversal of the field the linear term also reverses sign, a hallmark of piezomagnetism. The switching phenomenon persists during subsequent field reversals, demonstrating robust magneto-elastic memory. This is the first example of piezomagnetism in an actinide spin system and the magnetoelastic memory loop here is nearly an order of magnitude wider in field than those previously observed, making UO_2 the hardest piezomagnet known. The unusually strong correlations between the magnetic moments in U-atoms and lattice distortions are a direct consequence of the non-collinear symmetry of the magnetic state.

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Dynamics of hard nanoparticles in organic matrix studied by Mössbauer spectroscopy

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Nanoparticles of $CuFeS_2$ (chalcopyrite) were embedded in an organic matrix as isolated particles one from another. ^{57}Fe transmission spectra were obtained in the temperature range $80 - 240K$. A dramatic drop of the isotropic recoilless fraction is observed versus temperature due to the particle rattling in a cavity of the matrix. Long range diffusion is observed above about $200K$ accompanied by localized long range motion in a "moving" cavity. The latter motion has very broad frequency range with low frequencies leading to the distinct broad component of the Mössbauer spectrum seen in addition to the diffusion broadened narrow component. Additional broadening of the broad component comes from the over-damped rattling of the particle. High frequency modes excited within particle via interaction with a thermal bath make discernible contribution to the second order Doppler shift never seen before by the Mössbauer spectroscopy to our best knowledge. The average size of the effective cavity was found as increasing linearly with temperature. A dramatic softening of the spring constant binding particle to the matrix was found versus increasing temperature.

Superconductivity in U-Pt system with low Pt concentrations ($\leq$ 15 at.%)

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It has been reported that Pt metal has only about $2-5$ at.% solubility in the cubic γ-U phase. Moreover, there is no report on the basic thermodynamic properties of the U-Pt system with low Pt concentrations. In our study, by using the splat-cooling technique with a cooling rate better than 10^6 K/s, we could extend a higher solubility of Pt metal in γ-U to at least 15 at.%, and stabilize this cubic γ-U phase down to low temperatures. We have investigated the low-temperature properties of U-15 at.% Pt splats in the temperature range of 100 mK - 300 K, as well as of the as-cast bulk sample (the precursor of the splat) and the annealed bulk one. All investigated alloys become superconducting below 1.1 K. U-15 at.% Pt splat has a lowest T_c (= 0.61 K) among all investigated U-T splats (T = Mo, Nb, Zr, Pt) having the γ-U structure. The H-T diagram of U-15 at.% Pt splat does not fit well to the Ginzburg-Landau theory. The specific-heat jump at T_c amounts less than 20% the estimated value from the BCS theory.

Types of magnetic order in iron-based superconductors parent compound PrFeAsO studied by Mössbauer spectroscopy

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The $PrFeAsO$ is a parent compound of the iron-based superconductors belonging to the '1111' family. It was studied by Mössbauer spectroscopy in temperature range $4.2 - 300K$. An itinerant $3d$ magnetic order develops at about $165K$ and it is accompanied by an orthorhombic distortion of the chemical unit cell. A complete longitudinal $3d$ incommensurate spin density wave (SDW) order develops at about $140K$. A region between above two temperatures is called a "nematic" phase with poorly understood microscopic magnetic properties. Significant part of SDW along propagation direction is almost free of the ordered electronic spins in the "nematic" region. Hence, it is likely that somewhat "mysterious nematic" phase is a region of incoherent spin density wavelets typical for a critical region. This region is exceptionally broad on the temperature scale (more than $20K$) and the reasons for that could be strong scattering of the electronic spins on the large localized moments of praseodymium with significant orbital contribution. Praseodymium orders magnetically at about $12K$ leading to the substantial transferred field on iron nuclei due to the large orbital contribution to the magnetic moment. A reorientation of the praseodymium magnetic moments was reported at still lower temperatures.

Exotic Spin-Orbital Physics in Hybrid Oxides

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Strong Coulomb interactions in transition metal oxides suppress charge fluctuations and lead to superexchange with spin-orbital entanglement [1]. Here we consider two situations for neutral defects at the transition metal sites: (i) orbital dilution for $3d^3$ (Mn^{4+}, Cr^{3+}) impurities in $(Ca,Sr)_2RuO_4$, and (ii) charge dilution due to hole-doublon pairs for $3d^2$ doping. The spin-orbital superexchange concerns host d^4-d^4 (J) and hybrid d^4-d^n (J') bonds ($n=2,3$). The overall consequences of doping for the spin-orbital order in the host depend on the coupling on the hybrid bonds and on Hund's exchange at impurity ions. The orbital dilution (i) modifies locally or even globally spin-orbital order [2]. One finds that around impurities host orbitals change from inactive ones to orbital polarons for increasing J'/J. For charge dilution (ii) intersite excitations generate $T_i^+T_j^+$ terms responsible for simultaneous hole-doublon excitations which enhance orbital quantum fluctuations. Our findings are expected to be of importance for future experimental and theoretical studies of correlated oxides with $3d$ impurities of different valence.

Work supported by NCN Project No. 2012/04/A/ST3/00331.

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Charge-ordered stripes in the narrow-bandwidth limit of the extended Hubbard model

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Various charge ordered states are relevant to a broad range of important materials, including manganites, cuprates, magnetite, several nickel, vanadium and cobalt oxides, heavy fermion systems and numerous organic compounds. The extended Hubbard model is one of the simplest models that captures the interplay between strong correlations and charge-ordering effects [1-6]. It has been found that the model can describe the insulator-metal transition between phases with long-range charge-order [1,2]. We present studies of the model with both (i) the effective on-site interaction U and (ii) the intersite density-density interactions W_{ij} (nearest-neighbor W_1 and next-nearest-neighbor W_2) beyond the standard two-sublattice assumption [3-6]. We investigate in details the effects of next-nearest-neighbor interactions on phase diagrams of the model in different limits and we show that charge-stripes can occur for repulsive $W_2 > 0$ in a case of $W_1 > 0$ (as well as for $W_1 < 0$) [7]. In addition, we discuss the properties of several stripe charge-ordered phases, which can be stabilized by longer-range density-density interactions on various three dimensional lattices (e.g. SC and BCC lattices).

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Low-energy electronic structure of UPd_2Al_3, UGa_2, FeO and NiO

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There is a long debate on the role played by d and f electrons in the iron-group and uranium compounds. They are itinerant or localized being described by band models or crystal-field-based models. From experimental point of view there are some evidence for band description. In this presentation we will analyze experimental evidence for the localized behavior with the existence of the low-energy electronic excitations close to the Fermi level. Scientifically important is whether heavy-fermion excitations in UPd_2Al_3, for instance, are of the charge or of neutral character involving only the spin. In correlation with the low-energy, below 20 meV, electronic structure we will discuss the formation of the magnetic moment and the magnetic anisotropy revealed in high-field magnetization curves.

UPd_2Al_3 exhibits superconductivity coexisting below T_{sc} of 2 K with the antiferromagnetic state (T_N = 14 K) with a substantial U magnetic moment. UGa_2 is unique uranium compound being ferromagnet with T_c =125 K.

FeO and NiO are prototypes of Mott insulators being insulators despite of open 3d shell. In all mentioned compounds we will derive spin and orbital moment. Our studies reveal substantial orbital moment in FeO and NiO pointing the importance of the spin-orbit coupling in $3d$ ions despite of a common text-book knowledge that the orbital-moment is quenched in $3d$-ion compounds (due to the weakness of the spin-orbit coupling). We have found that the small off-cubic distortions determine the direction of the Fe/Co moment.

Distinctive response of many-body localized systems to strong electric field

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The many–body localized (MBL) systems together with the Anderson insulator might represent the only *generic* solid–state systems which do not thermalize in the thermodynamic limit and, therefore, may be used to store quantum information. We study systems which are close to or within the MBL regime and are driven by strong electric field. In the ergodic regime, the disorder extends applicability of the equilibrium linear–response theory to stronger drivings, whereas the response of the MBL systems is very distinctive, revealing currents with damped oscillations. The oscillation frequency is independent of driving and the damping is not due to heating but rather due to dephasing. The details of damping depend on the system's history reflecting nonergodicity of the MBL phase, while the frequency of the oscillations remains a robust hallmark of localization. We show that the distinctive characteristic of the driven MBL phase is also a logarithmic increase of the energy and the polarization with time.

Critical Phenomena in Condensed Matter Physics: a simple overview

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In this lecture I will briefly recall the evolution during the last century of the reduction schemes used in Condensed Matter Physics to describe the properties of macroscopic systems arising as a consequence of the interaction among the elementary objects, which depending on the problem under consideration can be atoms, electrons, spins,âĂę Particular emphasis will be given to the concept of quasi-particles and the related many body techniques for solving approximately the corresponding dynamics and reduce an interacting system into a gas of excitations. Staring from the Landau theory of Normal Fermi Liquid for the electrons in metals and for the normal phase of Helium3, I will introduce the instabilities of Fermi systems towards symmetry broken phases like superconductivity, superfluidity, magnetism. Within the presentation of critical phenomena, it will be apparent that all the standard perturbation approaches used up to the sixties in many body systems cease to be valid. Near the instability infinitely many degrees of freedom have to be considered simultaneously. Emergent properties of the system seems to put in crisis any reductionist approach. The introduction of the Renormalization Group in critical phenomena overcomes this crisis and, contrary to a bad popularization, the reductionism scheme from small and simple to the macroscopic and complex has not been put in crisis. Complexity and the specific reductionism at the birth of the renormalization group approach to critical phenomena are presented. Reductionism has been appropriately used through a suitable contraction of variables via the elimination of the irrelevant variables and a subtle procedure of filtering those variables appropriate to the description of the problem under discussion without solving the specific dynamic of each system.

The Black Hole in a piece of Copper Rust

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It appears that big progress in science typically happens when it is realized that seemingly unrelated subjects turn out to have a common ground. I had the luck to just stumble in such a constellation as related to two established main streams in physics. On the one hand, string theory as a fanciful mathematical machine building affair, desperately looking for empirical context. On the other hand, condensed matter physics with its strongly interacting electron systems, devoid of powerful equations. I will tell the story how these found each other, merging in an exciting new reality where one can study fanciful forms of Hawking radiation in mundane pieces of earthly rocks.

	Thursday, 29/09	
8^{00}- 9^{00}	**breakfast**	**Page in book of abstracts**
chair:	***Z. Kąkol***	
9^{00}- 9^{40}	M. Giersig: Magnetic Nanoparticle Superstructures	51
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10^{20}- 11^{00}	T. Domański: From superconductivity to electronic correlations	53
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13^{30}- 15^{00}	**lunch**	
	excursion/ free time	
20^{00}- 22^{00}	**conference dinner**	

Magnetic Nanoparticle Superstructures

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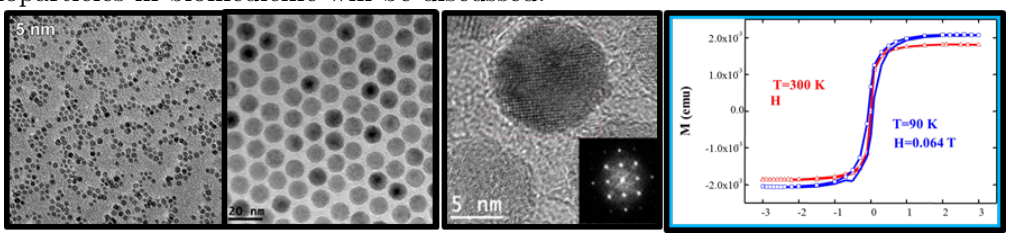
Nanotechnology allows us to manipulate matter at the level of individual atoms and produce materials with new properties that differ from their counterparts in the solid state. In this lecture, we will discuss our study about the advances in the preparation of magnetic nanoparticle superstructures by use of wet chemistry and of the physical method (1-5). In the first part I will focus on the preparation of monodisperse superparamagnetic nanoparticles as well as on the creation of two and three dimensional particles assembling. In the second part representative examples of applications of such nanoparticles in biomedicine will be discussed.



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Kondo effects in quantum dots: A tutorial overview

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Quantum dots are grateful objects for testing fundamental physical issues, e.g. entanglement of electrons, the Kondo type correlations, non-Fermi liquid properties and quantum phase transitions. The lecture focusses on various aspects of the Kondo resonance. I start with a single quantum dot and formation of the Kondo singlet accompanied by the Abrikosov-Shul peak in the density of state. It is manifested itself an increase of the conductance when temperature is lowered (in contrast to bulk metals with magnetic impurities where the resistance increases in low temperature) [1]. I show interplay of the Kondo resonance with quantum interference processes, for example with the Fano resonance and the Aharonov-Bohm effect [2]. Next, more complex situations with the spin $S > 1/2$. In this case one can observe the underscreening Kondo effect when conducting electrons cannot fully screen the magnetic moment of the impurity. The triple quantum dot system is interesting object for research, because varying gate potentials one can observe quantum phase transitions between different many-electron states with $S = 0$, $S = 1/2$ and $S = 1$, with the regular Fermi liquid and singular-Fermi liquid phases [3]. The lecture presents also recent experiments on the overscrerened Kondo effect in quantum dots, i.e. on the two-channel Kondo effect which involves two sources of electrons that form two separate electron channels [4].

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From superconductivity to electronic correlations

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Superconductivity spread on nanoscopic objects by the proximity effect reveals a plethora of new and amazing phenomena. For instance, in heterojunctions with the correlated quantum impurity embedded between the metallic and superconducting electrodes the induced pairing cooperates with the Coulomb repulsion, *enhancing* the Kondo effect. Such counter-intuitive phenomenon occurs near the quantum phase transition from the doublet to singlet configurations [1,2]. In more complex 3-terminal structures, the same mechanism implies the *universal scaling* of the Kondo temperature vs Josephson phase [3]. The 3-terminal structures allow for the strong *non-local* charge [4] or thermoelectric [5] transport and can be efficient source of the spatially entangled electrons. I shall highlight these and other related issues.

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Ferromagnet-superconductor nanosized heterostructures for basic research and applications

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Ferromagnet/superconductor heterostructures are an attractive model system for studying the interaction between magnetism and superconductivity in low-dimensional structures. In this work we present results of the recent studies of the heterostructures composed of alternating ferromagnetic $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) and superconducting (SC) $YBa_2Cu_3O_7$ (YBCO) layers. We have observed evident influence of the magnetic LSMO layer on SC properties of the adjacent YBCO layer. The Nernst effect was studied in the mixed state revealing the characteristic temperature dependence of the Nernst signal which seems to be correlated with the variation of the upper critical field. Pseudogap (PG) properties of the heterostructures have been derived from the analysis of the excess conductivity, σ', and discussed within the local pair (LP) model. This model is based on the assumption that in cuprate high-T_c superconductors, paired fermions are formed below the characteristic temperature $T^* \gg T_c$ resulting in PG opening. Near T_c, the $\sigma'(T)$ dependence was found to be perfectly described by the Aslamasov-Larkin and Hikami-Larkin fluctuation theories, suggesting the presence of SC fluctuations in a relatively large (up to 15 K) temperature range above T_c.

Fermi surface topology and quantum size effect in bilayer graphene

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Bilayer graphene (BLG) rises as one of top-tier candidates for post-silicon electronics, mainly because its tunable band gap. Unlike for a monolayer, a low-energy excitations of which are correctly characterized by the Fermi velocity $v_F \approx 10^6\,\mathrm{m/s}$, minimal description of BLG usually involves three microscopic parameters [1]: The nearest-neighbor intralayer hopping integral ($t_0 = 3.16\,\mathrm{eV}$), the direct interlayer hopping integral ($t_\perp \approx 0.4\,\mathrm{eV}$), and the skew-interlayer hopping integral ($t \approx 0.1 - 0.3\,\mathrm{eV}$). The first two are determined with a good accuracy, as they are directly related to the physical quantities which are the asymptotic Fermi velocity v_F and the low-energy effective mass $m_{\mathrm{eff}} = 0.033\,m_e$ (with me the free electron mass). The third parameter is related to the so-called Lifshitz energy EL, defining the energy range ($-E_L < E < E_L$) in which the Fermi surface splits into a four element manifold for each valley, and is currently know with a limited precision. We describe theoretically a collection of physical effects, including the conductance and shot-noise evolution with the system size [2,3] and magnetic field [4], in which measurable quantities are strongly affected by skew-interlayer hoppings. A finite-system version of the Lifshitz transition is put forward and interpreted as a manifestation of the time-energy uncertainty relation.

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Silicene on metallic quantum wells

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Freestanding silicene, a silicon equivalent of graphene, is a two-dimensional material composed of Si atoms arranged in a honeycomb lattice. This material has been predicted to give rise to massless Dirac fermions. However, due to the preferred sp^3 bonding of silicon the freestanding silicene layer may not be easily realized in experiment. Therefore it must be grown on a substrate, where the interaction between silicene and the substrate cannot be neglected.

In this talk a recently proposed efficient way of tuning the silicene-substrate interaction will be presented. The idea utilizes quantum size effect in the substrate. As an example the silicene on ultrathin Pb(111) layers will be considered, and it will be demonstrated how the properties of silicene, including binding energy, properties of Dirac cone, magnitude of energy gap, can easily be modified and controlled by quantum well states. Moreover, a novel mechanism of protecting the Dirac particles from the influence of the substrate, associated with special arrangement of a part of Si atoms in silicene, will be discussed.

This work has been supported by the National Science Centre under Grant No. DEC-2014/15/B/ST5/04244.

Structural functionalization of silicene

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Silicene, a two-dimensional material composed of silicon atoms, is known as a counterpart of graphene. However, these materials differ slighly in the atomic structure as freestanding silicene exhibits low-buckling in the atomic scale while graphene is flat. They share many features such as honeycomb lattice, linear bands crossing at the Fermi level in tke K points of Brillouin zone and the related excellent conductivity. Their transport properties can easily be tuned by many external meanings e.g. strain, electric field or adatoms adsorption.

We give a systematic analysis of the silicene atomic and electronic structure under geometrical functionalization based on the first principles density functional theory calculations. We show how corrugation, uniform and nonuniform strain affects the silicene properties, in particular location and shape of the Dirac cone and the related anisotropy in the electron group velocity.

This work has been supported by the National Science Centre (Poland) under Grant No. DEC-2014/15/N/ST3/03816.

	Friday, 30/09	
8^{00}- 9^{00}	**breakfast**	**Page in book of abstracts**
chair:	***T. Domański***	
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9^{40}- 10^{20}	J. Zakrzewski: Many-body localization due to random interactions	62
10^{20}- 11^{00}	TBA	
11^{00}- 11^{30}	**coffee/tea**	
12^{30}- 14^{00}	**lunch / departure**	
14^{00}	departure by bus: Zakopane	

Nontrivial properties of fermions "anomaly" coupled to classical continuous degrees of freedom

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We consider a coupled boson-fermion model in two dimensions, that describes itinerant fermions hybridizing with localized bosons composed of pairs of tightly bound opposite-spin fermions. We trace out the fermionic degrees of freedom and perform a Monte Carlo simulations for the effective classical Hamiltonian of boson phases. We find that fermions generate an effective long-range temperature-dependent boson-boson coupling leading to a finite phase stiffness. With increasing temperature the stiffness drops to zero and the bosonic subsystem undergoes the Kosterlitz-Thouless transition. It is interesting that also the fermionic subsystem has nontrivial properties, what results from the interactions with the classical phases. At low temperature the phases are uniform and the fermions form a BCS state independently of the strength of the boson-fermion coupling. However, at higher temperature the fermions interact with inhomogeneous distribution of the boson phases. Depending of the coupling they form a metallic state, Anderson insulator or a disordered bosonic insulator.

Many-body localization due to random interactions

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The possibility of observing many body localization of ultracold atoms in a one dimensional optical lattice is discussed for random interactions. In the non-interacting limit, such a system reduces to single-particle physics in the absence of disorder, i.e. to extended states. In effect the observed localization is inherently due to interactions and is thus a genuine many-body effect. We concentrate on bosons but a similar model works also for fermions in an optical lattice. In the system studied, many-body localization manifests itself in a lack of thermalization visible in temporal propagation of a specially prepared initial state, in transport properties, in the logarithmic growth of entanglement entropy as well as in statistical properties of energy levels. The latter obey faithfully the semi-Poisson level spacing distribution in the localized regime.

Posters

Influence of doping on charge modulation at superconducting transition in iron pnictides studied by Mössbauer spectroscopy

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Iron-based superconductors $Ba_{0.6}K_{0.4}Fe_2As_2$ belonging to '122' family (critical temperature $T_c = 38K$) and $SmFeAsO_{0.91}F_{0.09}$ belonging to '1111' family ($T_c = 47K$) were investigated by Mössbauer spectroscopy versus temperature with particular attention paid to the region of superconducting transition. Spectra display quasi-continuous distribution of quadrupole doublets in the whole temperature range. A distribution is caused by the spatial modulation of the electric field gradient, i.e., by the electric field gradient wave (EFGW), the latter being consequence of the incommensurate modulation of the charge density on the iron nuclei, i.e., the charge density wave (CDW). Shape and amplitude of EFGW and CDW are strongly perturbed at the superconducting transition. Namely, all modulations are strongly changed at critical temperature due to the superconducting gap opening and subsequent formation of Cooper pairs. However dispersion of the charge density and EFGW shape behave in the opposite ways for these two superconductors. These differences follow the manner of doping above compounds to achieve superconductivity. The '122' superconductor is hole doped, while the '1111' superconductor is electron doped. Hence, the Fermi surface moves opposite way for above cases.

Influence of intercalation-type on superconducting properties of iron chalcogenides studied by Mössbauer spectroscopy

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The iron-chalcogenide superconductors $Cs_xFe_{2-z}Se_2$ ($T_c = 25K$) and $Li_x(C_5H_5N)_yFe_{2-z}Se_2$ ($T_c = 40K$) have been investigated by Mössbauer spectroscopy. For both compounds in the as-prepared and annealed state multi-component Mössbauer spectra were obtained. A non-magnetic component emerging due to the iron located in the unperturbed $Fe-Se$ sheets is assumed to be responsible for superconductivity. Remaining components were found to be magnetically ordered even at room temperature. Thus, apparently (x-ray patterns!) almost single phase superconducting $A_xFe_{2-y}Se_2$ samples are in fact, on the microscopic scale, multi-phase materials with superconducting and magnetic regions spatially separated. Additional annealing leading to ordering of the iron vacancies within $Fe-Se$ sheets was necessary to achieve superconductivity. Larger distance between the $Fe-Se$ layers as obtained by the intercalation with $Li_x(C_5H_5N)$ in comparison with Cs, leads to an increase of the critical temperature and the superconducting volume fraction in agreement with the two-dimensional superfluid density hypothesis.

STM/STS and magnetoresistance studies of $Bi_{1.96}Mg_{0.04}Se_3$ single crystal.

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We present the results of magnetoresistance and STM/STS of $Bi_{1.96}Mg_{0.04}Se_3$ single crystal. The aim of the studies was to confirm nontrivial electronic states topology of this material and to look for its possible signatures at low temperatures. The single crystal was synthesized via the Bridgman method from initially 5N purity elements deoxidized and purified by multiple vacuum distillations until 7N purity was reached. Magnetoresistance measurements were carried out in temperature range from 20 mK up to 30K in magnetic fields up to 14T by standard four probe technique with SR 7270 lock-in amplifier. The STM/STS measurements were performed in UHV STM system with RHK scanning head at room temperature. The hexagonally ordered atomic structure attributed to (001) plane is revealed, with STS results suggesting linear dispersion relation of the surface states. The results are compared to the first-principles density functional theory electronic structure calculations supporting both, STM and STS, observations.

Thermodynamic properties of the extended Hubbard model with pair-hopping interaction in the limit of very narrow bandwidth

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The Penson-Kolb-Hubbard model is one of the conceptually simplest phenomenological models for studying correlations and for description of superconductivity in very narrow-band systems. The relevant question is how accurate the standard broken-symmetry Hartree-Fock mean-field approximation is when applied to the on-site term U (for both repulsive and attractive U). We present phase diagrams and investigate the thermodynamic properties of the model derived within the Hartree-Fock approach in the narrow-bandwidth regime. The results are compared with those exact ones in the atomic limit for the limit of high dimensions. In particular, we analyze the evolutions of thermodynamic potentials and order parameters (with special attention to those of the superconducting phases) as a function of the model parameters. Our investigation of the general case, for relevant values of the interaction parameters and electron concentration, shows that results obtained within both approaches are consistent, at least in the low temperature regime.

Stable high-temperature paramagnons in a dimerized antiferromagnet near quantum criticality

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Inelastic neutron scattering (INS) experiments [1] on a dimerized antiferromagnet $TlCuCl_3$ have revealed a sharp amplitude (or Higgs) mode close to the pressure-induced quantum phase transition below the Néel temperature T_N. The width to mass ratio (FWHM/m) of magnetic excitations above T_N is approximately equal to that of the amplitude mode for $T \to 0$ in the range of pressures, which signals remarkable robustness of paramagnons to thermal damping [2].

We carry out a study of masses and lifetimes of magnetic excitations across quantum and classical transitions, within the framework of phenomenological Ginzburg-Landau model using the hybrid modified minimal subtraction + thermal renormalization group method. We demonstrate that FWHM/m of the paramagnons above T_N scales with the $T \to 0$ FWHM/m of the amplitude mode, with a proportionality factor ≈ 1, which is consistent with the available INS data. Two principal factors, responsible for the latter behavior, are identified: (i) the emergence of thermal mass scale which leads to a non-analytic form of paramagnon decay rate, and (ii) renormalization of the multi-magnon interactions by thermal fluctuations.

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Degenerate Anderson lattice model: Modified Schrieffer-Wolff transformation, exchange interactions, and real space paring

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We apply the canonical perturbation expansion to the orbitally degenerate periodic Anderson model in direct space, similar to that in the nondegenerate case [1]. We assume orbital degeneracy of both c and f-levels ($l = 1, 2$) and add terms: the Hund's rule coupling and the Coulomb interaction between f-orbitals. The transformation is carried up to the second order by a modified Schrieffer-Wolff transformation: we separate the part of hybridization term responsible for the high-energy processes (in the simplest case the triplet state in the intermediate state) and replace it with the virtual processes in higher orders.

The obtained Hamiltonian for the case when average number of f-electrons per site n^{f} is $1 \leq n^{\mathrm{f}} \leq 2$ contains both the Kondo (f-c) and the f-f pairing interactions, as well as a residual hybridization responsible for the heavy-quasiparticle formation. This effective Hamiltonian can be used to analyze the magnetic or the paired states, as well their coexistence in heavy-fermion systems.

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C-axis-polarized phonons in $HgBa_2CuO_{4+\delta}$ studied by inelastic X-ray scattering

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The phonon spectrum of optimally doped single crystalline high-T_c superconductor $HgBa_2CuO_{4+\delta}$ (Hg1201) was measured via inelastic X-ray scattering (IXS). The aim was to discern the possible phononic contribution to the magnetic order and the associated excitations in the pseudogap phase revealed by polarized inelastic neutron scattering (INS) [1,2]. This magnetic order, found in a process of the wider search of the pseudogap origin, was centered at the Brillouin zone center ($q = 0$) and the corresponding excitations were observed at energy transfers of 35 and 53 meV, and distinctly different from the well-known spin fluctuations near the antiferromagnetic wave vector $\mathbf{q}_{\mathrm{AF}} = (1/2, 1/2)$. Although spin-flip neutron scattering experi-ments suggested their magnetic origin, phononic contribution could not be decisively rejected by INS; our IXS experiment was supposed to check this conjecture. Additionally, we wanted to further characterize the phononic spectrum of Hg1201.
We have tracked the c-polarised phonons with momentum transfer $Q = (-0.5\,0.5\,7)$ and $Q = (-0.3\;0.3\;7)$. We have found: a) a clear anomalous behaviour for $T = 20\,\mathrm{K}$ and close to q = (1/2 1/2 0) (possibly due to spin fluctuations); b) some difference between $T = 20\,\mathrm{K}$ and $T = 100, 250\,\mathrm{K}$ for low energy ($E = 11\,\mathrm{meV}$) phonons (with momentum transfer $Q = (-0.3\;0.3\;7)$); c) some increased intensity around 75 meV, again observed mainly for the momentum transfer $Q = (-0.3\;0.3\;7)$.
The absence of phonons at the energies where the excitations in INS were found supports the scenario of their magnetic origin.
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Ion beam mixing effect in magnetite thin films

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Magnetite is one of the oldest known magnetic material and nowadays it is considered as a promising candidate for spintronic applications at room temperature.
The objective of this work is investigation of the structure and properties of the magnetite thin film systems with single- and bi-layer structure and with different layer thicknesses. The work is focusing to studying the ion beam mixing effect and the interdiffusion process.
The film chemical composition, layer thicknesses and structure in the as-grown state, after a post annealing treatment and after being modified by Ar+ and Kr+ion beam have been investigated by means of Rutherford back-scattering and RBS- channeling. For the data evaluation, the computer code SIMNRA was employed.
Our analysis of the effect from post-annealing and ion irradiation indicates that Mg and Fe diffusion leads to a formation of a large interface zone having a spinel and/or wustite formula. However the pure magnetite layer on the surface can be well preserved upon irradiation with small doses.

Characterization and modification of Fe and Pd thin films

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We are interested in characterizing the stability of Fe and Pd thin films with the (001) texture grown on an amorphous substrates like a SiO_2/Si(001) against thermal annealing and high-energy ion bombardments.
Thin films consisted of 10nm Pd/100nm SiO_2/Si(001) and 10nm Fe/100nm SiO_2/Si(001) have been prepared by a thermal evaporation method at a working pressure in the range of 10^{-6} Pa.
We have performed the investigations on the film in three different states: 1) as-deposited state, 2) after a rapid post-annealing at 600^0C for 90s and 3) after irradiation by 1MeV Ar^+ beam with different ion fluencies. The chemical composition and layer thickness of the films have been definied by a Rutherforfd Backscattering Spectrosopy (2MeV He^+ ion beam, scattering angle of 171^0). For the data evaluation, the simulation program SIMNRA was employed. To confirm the data obtained from the RBS measurement, the X-ray reflectivity (XRR) measurements have been performed. To image the surface structure after a post- annealing the Atomic Force Microscope (AFM) and the Scanning Electron Microscope (SEM) have been used.

The extended states in disordered 1D systems in the presence of the generalized N-mer correlations

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We have been investigating the problem of the Anderson localization in a disordered one dimensional tight-binding model. The disorder is created by the interaction of mobile particles with other species, immobilized at random positions. We introduce a novel method of creating correlations in the optical lattices with such a kind of disorder by using two different lattices with commensurate lattice lengths to hold two species of the particles. Such a model, called the generalized random N-mer model leads to the appearance of multiple extended states in contrary to a localization of all states usually expected in one dimension. We develop a method, based on properties of transfer matrices which can be used to determine the presence of extended states and their energies for that class of correlations. Analytical results are compared with the numerical calculations for several cases which can be realized in cold-atom experiments.

EPR signal as the fingerprint of strong electron correlations in hexagonal 4H-$SrMnO_3$

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The EPR signal, revealed at the vicinity of T_N and in the paramagnetic region in 4H-$SrMnO_3$ [1], has been explained as related with the doublet ground state originating from the $^4A_{2g}$ subterm of the Mn^{4+} ion. Our calculations, taking into account the spin-orbit coupling and the crystal-field interactions with a trigonal distortion, reproduce the doublet ground state which is characterized by magnetic moment of $\pm$ 0.975 μ_B in very good agreement with experimental value of $\pm$ 0.983 μ_B [1]. It confirms fundamental importance of the spin-orbit coupling and the orbital magnetism for description of $3d$ oxides [2,3]. We claim that the EPR result provides a strong argument for the existence in the 4H-$SrMnO_3$ crystal of the discrete atomic-like crystal-field states with the energy separation of part of meV. Within the same atomic-like approach we have managed to describe temperature dependence of the specific heat in the AFM and paramagnetic states including the λ-type peak at T_N.

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Superconductivity in La-based 1:2:2 d-electron silicides and germanides

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In the course of our systematic search for new unconventional superconductors among the RT_2Si_2 and RT_2Ge_2 compounds (where R stands for Y, Th, La, Lu or Sc, and T is a transition metal) we have synthesized and studied structural and low-temperature physical properties of the less known La-based silicides with Fe, Co, Ag and Au, and germanides with Fe, Co, Ni, Cu, Ag, Ir, Au, Ru, and Rh. X-ray powder diffraction experiments revealed that most of the compounds crystallize in the orthorhombic $ThCr_2Si_2$-type structure and only $LaIr_2Ge_2$ forms with the $CaBe_2Ge_2$-type unit cell. Magnetic, electric and thermal measurements performed in wide temperature and magnetic field ranges showed that only $LaCo_2Ge_2$ shows bulk superconductivity below about 2.1 K, while the other systems are non-superconducting metals at least down to 0.35 mK. We present detailed analysis of the superconducting state in $LaCo_2Ge_2$ together with the results of band structure and Fermi surface calculations performed using the FPLO method for all the compounds studied. We compare them with the data obtained for Y- and Th-based systems reported before.

The work was financed by the National Centre of Science (NCN, Poland) within a research grant no. 2014/13/B/ST3/04544.

Discrete low-energy electronic structure in $FeBr_2$ and $LaCoO_3$

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We have derived low-energy electronic structure of $LaCoO_3$ and $FeBr_2$ from analysis of magnetic and electronic properties. $LaCoO_3$ presents peculiar magnetic properties - its paramagnetic susceptibility violates Curie-Weiss law exhibiting a maximum at 100 K. $FeBr_2$ shows antiferromagnetism below $T_N = 14$ K visible by the λ-type peak. The magnetization curve shows a metamagnetic transition at 3.15 T and then the magnetization reaches a quite large value of 4.3 μ_B. These properties we have described within the Quantum Atomistic Solid State Theory (QUASST) by considering properties of the Fe^{2+} ions in $FeBr_2$ and Co^{3+} ions in $LaCoO_3$. Despite of very different crystallographic structures (hexagonal and cubic) anions form local octahedron which is only slightly trigonally-distorted in case of $FeBr_2$. 6 electrons in Fe^{2+} and Co^{3+} ions form strongly-correlated electronic system $3d^6$. We have derived low-energy electronic structure associated with the Fe^{2+} and Co^{3+} ions taking into account the relevant crystal-field parameters and the spin-orbit coupling. The nonmagnetic ground state of $LaCoO_3$ is effect of strong crystal field. Calculated by us electronic structure of $LaCoO_3$ is in nice agreement with EPR experiments which have confirmed the predicted existence of very thin localized crystal-field levels. The existence of very thin localized crystal-field levels in a $3d$ oxide is very surprised as modern theories predict the formation by $3d$ electrons very wide bands. Our studies on $FeBr_2$ reveal substantial orbital Fe moment pointing the importance of the spin-orbit coupling.

ARPES studies of $Fe_{1.02}Te_{0.65}Se_{0.35}$, $Fe_{0.95}Co_{0.09}Te_{0.67}Se_{0.33}$ and $Fe_{0.95}Ni_{0.06}Te_{0.64}Se_{0.36}$

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Single crystals of $Fe_{1.02}Te_{0.65}Se_{0.35}$, $Fe_{0.95}Co_{0.09}Te_{0.67}Se_{0.33}$ and $Fe_{0.95}Ni_{0.06}Te_{0.64}Se_{0.36}$ were studied by means of angle-resolved photoemission spectroscopy (ARPES) using He-I radiation at temperature of 18 K. The measurements revealed Fermi surfaces and band structure along Γ-M. Three hole pockets at the Γ point and one electron pocket at the M point were observed. In the cases of the undoped and doped systems we determined the Fermi surface volume for both electron and hole pockets. Band shifts related to doping were also estimated. According to a simple electron count the effect of Ni doping for $Fe_{0.95}Ni_{0.06}Te_{0.64}Se_{0.36}$ should yield a larger increase of electron concentration than Co doping in $Fe_{0.95}Co_{0.09}Te_{0.67}Se_{0.33}$. In contrast, the ARPES studies indicate that more electrons are transferred to valence band for the Co doped sample. Moreover, a clear shift of the hole pocket below the Fermi energy, which is observed in $Fe_{0.95}Co_{0.09}Te_{0.67}Se_{0.33}$ and $Fe_{0.95}Ni_{0.06}Te_{0.64}Se_{0.36}$, indicate that a Lifshitz transition is realized in these systems.

Acknowledgments

Transport properties of the samples were characterized by
V. L. Bezusyy and M. Z. Cieplak.

Valley filter in graphene Corbino disk in crossed electric and magnetic fields

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Using the transfer matrix in the angular-momentum space we investigate the quantum transport properties of a ballistic graphene in the Corbino geometry in the presence of crossed electric and magnetic fields. We show that currents corresponding to the two valleys, K and K', propagate along the p-n junction and are spatially separated. An anisotropic mass in the system allows one to create a valley filter by suppressing one of the valley currents.

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Different lattice geometries using synthetic dimension

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The possibility of creating different geometries with the help of an extra synthetic dimension in optical lattices is studied. Additional linear potential and Raman assisted tunnelings are used to engineer well controlled tunnelings between available states. The great flexibility of the system allows us to obtain different geometries of synthetic lattices with possibility of adding synthetic gauge fields.

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