Book of Abstracts

From Spins to Cooper Pairs: New Physics of the Spins

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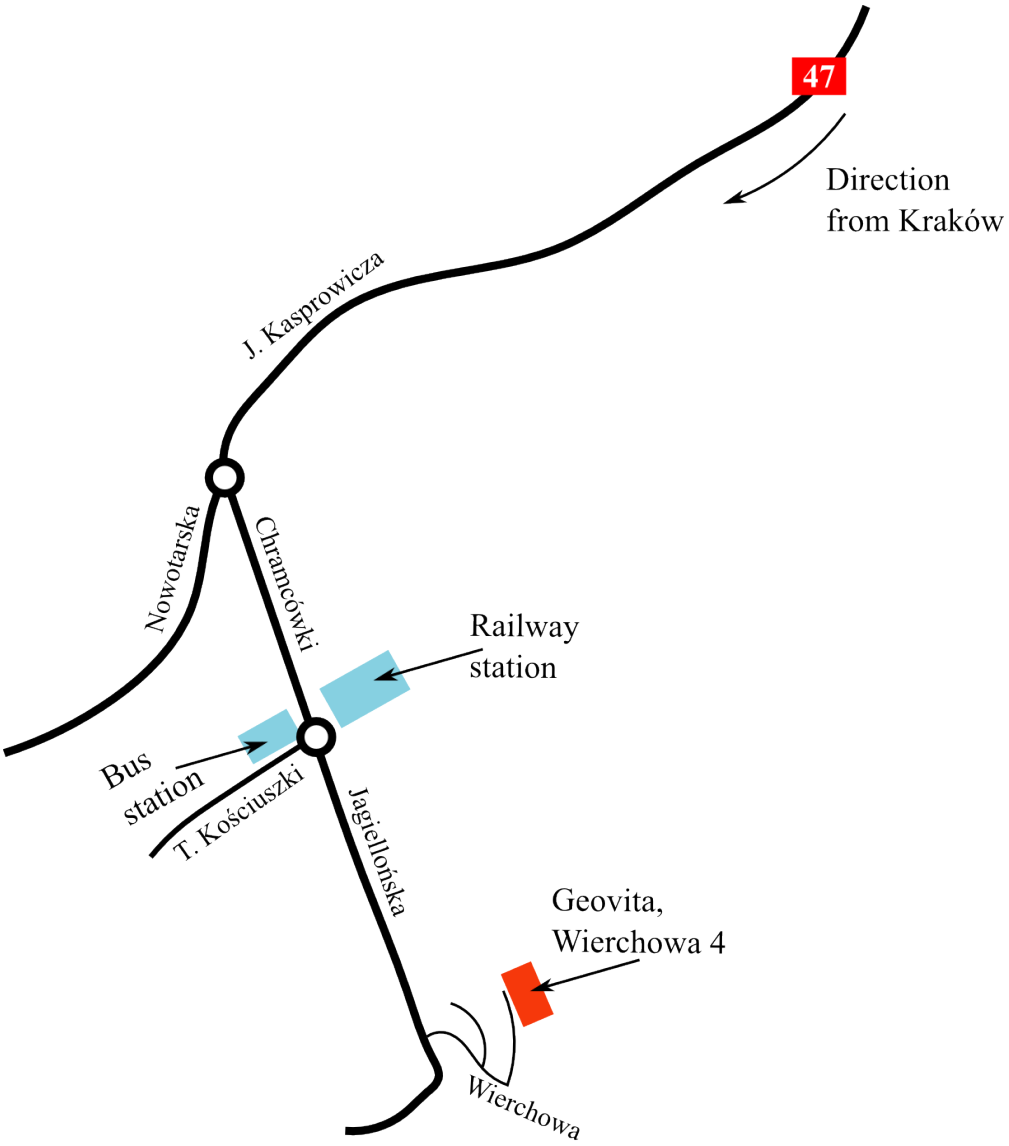
How to get there



Oral Presentations

Coexistence of superconductivity and antiferromagnetism in cuprates – study of extended t–J model

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We present the mean-field study of the t–J–U model in the context of the coexistence of superconductivity (SC) and antiferromagnetism (AF). The role of the spin-exchange coupling J and the next nearest hopping t' and t'' are examined. The coexistence (SC+AF) region exists for the sufficiently large Coulomb repulsion, and in the vicinity of the half-filled band, what corresponds well to experiments on cuprates. We checked that the effect of t' and t'' on the SC+AF region width is limited. Further, we discuss the effect of the electron hopping to the second (t') and to the third (t'') next neighbors on the strength of the superconducting phase. For small doping the effect is limited but for the overdoped region the presence of t' and t'' enhances the superconducting gap in a significant manner.

References:

[1] M. Abram et al., Phys. Rev. B **88**, 094502 (2013).

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Physics of nanowire spintronic devices

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Spintronics deals with the spin-polarized currents that are generated by spin filters and modified/controlled by spin transistors. The spintronic devices can be fabricated in either a planar (mesa) or vertical (nanowire) geometry. In my talk, I will discuss the physical background of the operation of the nanowire-based spin filters and spin transistors and present the results of computer simulations that show how the spin-polarized currents can be generated and modified in semiconductor nanowires.

The semiconductor spin filter exploits the spin Zeeman splitting of the electron energy levels in magnetic semiconductors and the resonant tunneling effect through the double-barrier structure. The results of computer simulations show that the nanowire consisting of GaN/GaMnN resonant tunneling structure can generate the current with the spin polarization that reaches 100% at 4.2 K and 75% at room temperature.

The semiconductor nanowire with the side gate electrode can operate as the field-effect spin transistor. The results of our calculations for the gate-controlled InAs nanowire demonstrate the spin transistor action induced by the Rashba spin-orbit interaction. We show that the appropriate tuning of the gate voltage generates the pronounced oscillations of the spin-polarized currents, which causes that both the spin-polarized current components can be switched on/off at different gate voltages, i.e., the spin transport is controlled by the all-electrical means. The computational results obtained for the room temperature are in a good agreement with the recent experimental data.

Quantum Critical Scaling of Fidelity in 2D BCS-like Models

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Extracting universal critical characteristics of systems from correlation functions in vicinities of their critical points is a non-trivial task. Derived in recent years scaling properties of ground-state fidelity opened an alternative, hopefully simpler, route to achieve this goal. This idea received a strong support from very recent studies of exactly diagonalisable 1D models, such as anisotropic XY model and Ising model in a transverse external field, and BCS-like models. Some anomalies have been found but typically the new method has appeared to be successful. By studying a 2D model with BCS-like pairing interaction we demonstrate that compared to 1D cases the situation is opposite. Thus the new method is unlikely to be successful in dimensions higher than one.

Entanglement, Kondo correlations and transport in a system of quantum dots

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We want present numerical renormalization group (NRG) studies of electronic correlations and entanglement in transport through a system of quantum dots. First, the results are presented for a single quantum dot described by an extended Anderson model which includes an assisted hopping term. The assisted hopping processes modify the coupling to the two-particle state, exponentially reduce the Kondo temperature, and strongly affect transport properties. Next we consider an artificial triangular molecule built of coherently coupled quantum dots in the presence of an electric field and magnetic flux, which affect spin correlations and entanglement. The magnetic flux destroys entanglement, it leads to circulation of spin supercurrents and spin delocalization. The electric field modifies superexchange correlations, breaks the triangular symmetry and leads to different local spin configurations. For some specific orientation of the electric field one can observe monogamy, for which one of the spins is separated from two others. Moreover changing the orientation of the electric field one can induce a quantum phase transition between different ground states with the total spin S=1/2 and S=1. Here the system exhibits two different behaviours: the fully S = 1/2 screened and underscreened S = 1 Kondo effect, which manifest themselves in different transport properties.

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The Gutzwiller Density Functional Theory

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Density Functional Theory (DFT) is the workhorse of electron structure theory. It reduces the genuine many-body problem to an effective single-particle theory that is readily treated numerically. However, electrons in narrow bands, e.g., 3d-electrons in transition metals and their compounds, require a more sophisticated treatment. Unfortunately, model Hamiltonians for correlated electrons often oversimplify the problem while, at the same time, they reintroduce the full complexity of the many-body problem. The Gutzwiller Density Functional Theory keeps the computational efficiency of existing DFT codes while it treats electronic correlations on the basis of Gutzwiller's variational many-body approach.

In my talk, I present a concise derivation of Gutzwiller DFT that is based on a multi-band Hubbard model with effective interaction parameters. In a first application to fcc nickel and bcc iron, I show that the main DFT shortcomings regarding lattice spacing, magnetic moment, bulk modulus, and Fermi-surface topology can be resolved in the Gutzwiller DFT. Lastly, I briefly discuss limitations and possible extensions of the method.

The effects of transition-metal substitutions in iron chalcogenides

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Doping of impurities into the host matrix is one of the efficient methods to modify the electronic properties of superconductors. Transition metal doping into Fe-site has been a subject of intense scrutiny in case of pnictide iron-doped superconductors. On the other hand, very few studies, and for very limited impurity contents, have been reported for chalocogenides, the other class of iron-doped superconductors. After a brief general introduction into the subject of impurity-induced effects in iron superconductors, we review here our recent research in this area, which provides first comprehensive study of the transport properties of single crystals of iron chalcogenides, substituted with transition metals, Co or Ni, up to a high impurity content.

Nanoindentation of Virus Capsids

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Molecular dynamics of proteins within coarse grained models have become a useful tool in studies of large scale systems. The talk will discuss two applications of such modeling. The first is a theoretical survey of proteins' resistance to constant speed stretching as performed for a set of 17134 simple and 318 multidomain proteins. The survey has uncovered new potent force clamps. They involve formation of cysteine slipknots or dragging of a cystine plug through the cystine ring and lead to characteristic forces that are significantly larger than the common shear-based clamp such as observed in titin. The second application involves studies of nanoindentation processes in virus capsids and elucidates their molecular aspects by showing deviations in behavior compared to the continuum shell model. Across the 35 capsids studied, both the collapse force and the elastic stiffness are observed to vary by a factor of 20. The changes in mechanical properties do not correlate simply with virus size or symmetry. There is a strong connection to the mean coordination number $< z >$, defined as the mean number of interactions to neighboring amino acids. The Young's modulus for thin shell capsids rises roughly quadratically with $< z >$ - 6, where 6 is the minimum coordination for elastic stability in three dimensions.

Heat and charge transport in a driven integrable system

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We study the transport of heat and charge in the $t-V-W$ model, a strongly interacting ring of spinless fermions, driven by a constant electrical field. In a closed system, the currents are nonmonotonic in time, due to the unbounded increase in temperature. When the heating effects are taken into account, for generic systems we recover the linear response expectations from the time evolved quantities. Integrable systems are characterized by ballistic transport and singular response functions, but the driving provides a regulator allowing the comparison to equilibrium estimates. Long time driving can also selectively lower the charge-current conductivity in integrable metallic systems, by suppressing conserved quantities at different rates, enhancing the thermoelectrical coefficients in a strongly nonlinear manner.

Strongly-Correlated Corner-Shared 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 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_{3-d} starting from the ferroelectric M=Ti (d^0), through colossal magnetoresistive and multiferroic M=Mn (d^3 and d^4), enhanced thermoelectric M=Co (d^6 and d^7), metal-insulator transitions in M=Ni (d^7) and finishing with the 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. 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. Perovskites exhibit unique oxygen non-stoichiometry, which can be used to sensitively vary the valence state of transition metals and, as such, control the properties; for example, Tc in high-temperature superconductors. However, oxygen non-stoichiometry itself can be regarded as a very 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.

Electrons' pairing versus long-range coherence from a boson-fermion perspective

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A number of recent experiments on the cuprate and pnictide superconductors provide a clear evidence that electron pairing survives well above T_c. This intriguing fact implies that formation of the electron pairs substantially differs from an onset of the long-range coherence. Their distinct signatures have been observed by the single particle spectroscopies and in the transport and magnetic properties. I will show that some of these features can originate from mutual feedback effects between the fermionic and bosonic degrees of freedom emerging in the strongly correlated electron systems.

Cooper Pairs in Subatomic Systems: To Spin or to Bosonize - That Is the Question

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It is well known that nuclear interactions are not only the strongest known in nature but also the most complex, combining the features of non-centrality and non-locality. And yet, experiments show that with no single exception the spins of the ground-states of all even-even nuclei (even number of protons, even number of neutrons) are equal to zero. This combined with the Kramers degeneracy accompanying nuclear systems as the result of the fact the nuclear Hamiltonian does not depend explicitly on time brings us to the conclusion that the nucleons (Fermions) 'live' in nuclei in couples with zero spin - thus forming effectively systems of bosons, the latter sometimes referred to as Nuclear Cooper Pairs.

We will describe the boson structure of the basically fermion-type subatomic systems avoiding all too specialised jargon. In particular we will describe the mechanisms which favour the presence of the subatomic bosonisation - but also the mechanisms which are its natural enemies. Among them: The Spinning - the term used often to describe the collective rotation of the subatomic systems the majority of which are non-spherical! We will also address the question: Why among about 3 000 nuclear species known today only hardly a dozen are those with the spherical shapes – all others being non-spherical or even strongly non-spherical. This property implies that the spatial orientation of the quantum subatomic systems can be defined - thus they can collectively rotate - and it will only be a matter of how fast? - to kill all the bosons!

Simulation of anomalous Hall effect in ultracold gases

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We study ultracold fermions trapped in a shaken two dimensional triangular lattice. We find that, a combination of interaction induced tunneling and shaking can result in an emergent Dice lattice along with controllable staggered magnetic flux and synthetic non-Abelian fields. Moreover, by tuning the staggered flux, we show that one can enter the regime of Quantum Anomalous Hall effect. Our results are reminiscent of Anomalous Hall conductivity in spin-orbit coupled Ferromagnets.

Heavy-tail distributions, Lévy noises and nonequilibrium stochastic thermodynamics.

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Superlinear and sublinear diffusional transport and nonexponential relaxation kinetics are ubiquitous in nature and have been observed and analyzed in a number of systems ranging from hydrodynamic flows and plasma physics to transport in crowded environment inside living cells and price variations in economy. Usually, a starting point of description of systems exhibiting anomalous transport properties involves use of continuous time random walk (CTRW) and fractional differential diffusion equations of the Fokker-Planck type (FFPE). Although both concepts turnt to be extremely powerfull in applications, there is still lack of full understanding of their links with first principles of statistical mechanics and thermodynamics. In the talk the issue of generalized susceptibility and response to external drivings in dynamic systems perturbed by non-Gaussian fluctuations will be discussed, pointing to the contemporary trials of extending Onsager's theory to far-rom equilibrium situations.

Influence of point defects on electronic structure and magnetic properties of YCo_2 compound

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The electronic band structures of YCo_2 systems with point defects are calculated using FP-LAPW method (Full Potential–Linearized Augmented Plane Wave) implemented in the WIEN2k code. The considered point defects are Nb and Ti substitutions and vacancies. Calculations show that the impurity atoms Ti and Nb strongly prefer to occupy the Y sites and the ferrimagnetic ground states are energetically more stable for YCo_2 systems with point defects in place of Y than in place of Co atoms. Theoretically predicted ferrimagnetic ground states for YCo_2 systems with Y atoms substituted by Ti and Nb find experimental confirmation in $Y_{0.9}Ti_{0.1}Co_2$ and $Y_{0.9}Nb_{0.1}Co_2$. The calculated reduction of the magnetic moment on Co for systems with point defects on Co agrees with experimental results for $YCo_{1.9}Ti_{0.1}$. This paper is continuation of work published by the same group of authors [Śniadecki et al. *J. Appl. Phys.* **115** (2014) 17E129].

Quantum phase transitions, ground-state correlations and fidelity in BCS-like models

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We study ground-state correlation functions in one- and two-dimensional models of interacting spinful fermions – BCS-like models, which exhibit continuous quantum phase transitions. The considered models originate from a two-dimensional model of d-wave superconductivity proposed by Sachdev. Due to the exact diagonalizability of the considered models, in any dimensionality and for any twisted boundary conditions, exact phase diagrams, with several kinds of quantum critical points, are constructed and closed-form analytic expressions for two-point correlation functions are obtained. In one- and two-dimensional cases we provide analytic expressions for the asymptotic behavior of those correlation functions at large distances and in neighborhoods of quantum critical points, in particular explicit expressions for correlation lengths and the values of universal critical indices ν that characterize the divergence of correlation lengths on approaching critical points. Specific scaling properties of correlations functions with respect to parameters of underlying Hamiltonians are revealed. The obtained results are used to study quantum fidelity approach to continuous quantum phase transitions.

Unconventional superconductivity in the Hubbard and t-J models: Gutzwiller wave function solution

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The superconducting phase of the Hubbard and t-J models is analyzed within a novel method called diagrammatic expansion for Gutzwiller wave function (DE-GWF). The lowest order of the method reproduces analytically the Gutzwiller Approximation results. With the increasing order the results of a truncated DE-GWF method converge to those of the variational Monte Carlo approach.

We obtain agreement with the experimental results: (i) the superconducting gap at the Fermi surface deviates from the $d_{x^2-y^2}$-wave symmetry; (ii) the nodal Fermi velocity is almost constant as a function of doping; (iii) the superconducting transition is driven by the kinetic-energy lowering for strong interactions.

Our method does not suffer from finite-size limitations, which allows us to study the Fermi surface deformations, i.e. nematic ("Pomeranchuk") phases, as well as their coexistence with superconductivity. An extension of the DE-GWF method to periodic Anderson model and to multiband systems is also feasible.

The work was supported by the Foundation for Polish Science under the "TEAM" program, as well as by the Ministry of Science and Higher Education under Grant No. 0171/IP3/2013/72.

Graph theory with Python: selected algorithms and applications

A. Kapanowski

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Graph theory is the study of *graphs*, which consist of some objects (nodes) and links between them (edges). Graphs can be used to model many types of relations and processes in physical, biological, social, and informations systems.

We would like to present a Python language library for the creation, manipulation, and study of graphs. The library includes a growing number of standard graph algorithms with a unified interface. The computational efficiency of implemented algorithms is confirmed by many tests. On the other hand, the source code can be read as a pseudocode in order to study algorithms. The unique features of Python are utilized: readable syntax, high level dynamic data types, exception-based error handling, and extensive standard libraries.

Basic features of the library are presented by means of the depth-first search algorithm and topological sorting. Some other problems from graph theory and their applications will be discussed: graphs coloring, Hamiltonian graphs.

$(H_2)_n$ molecule system with an *a*b initio optimization of wave functions in correlated state: Electron–proton couplings and intermolecular microscopic parameters

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The hydrogen molecules $(H_2)_n$ are analyzed with electronic correlations taken into account between the $1s$ electrons in an exact manner. The optimal single-particle Slater orbitals are evaluated in the correlated state of H_2 by combining their variational determination with the diagonalization of the full Hamiltonian in the second-quantization language. All electron–ion coupling constants are determined explicitly and their relative importance is discussed. Sizable zero-point motion amplitude and the corresponding energy are then evaluated by taking into account the anharmonic contributions up to the ninth order in the relative displacement of the ions from their static equilibrium value. The applicability of the model to the solid molecular hydrogen is briefly analyzed by calculating intermolecular microscopic parameters for $(H_2)_n$ rectangular configuration, as well its ground state energy. The present work is an extension of the earlier ideas [1].

References:

[1] A. P. Kądzielawa, A. Bielas, M. Acquarone, A. Biborski, M. M. Maśka and J. Spałek, arXiv:1405.1577 (2014);

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Anderson-Kondo lattice Hamiltonian from the Anderson-lattice model: A modified Schrieffer-Wolff transformation and the effective exchange interactions

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We derive the Anderson-Kondo lattice model by applying canonical perturbation expansion for the Anderson-lattice model in direct space. The transformation is carried out up to the fourth order by a modified Schrieffer-Wolff transformation: we separate the part of hybridization term responsible for the high-energy processes (involving the largest in-the-system intraatomic Coulomb interaction between f electrons) and replace it with the virtual processes in higher orders. The higher-order processes lead to three seperate exchange interactions. The obtained Hamiltonian contains both the Kondo (f-c) and the superexchange (f-f) 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. The magnitudes of both the Kondo exchange and the superexchange integrals are estimated as a function of bare hybridization magnitude.

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Clean Limit Superconductivity and Weak Itinerant Ferromagnetism in Y_9Co_7

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The paper presents new measurements of electrical resistivity, susceptibility and magnetization for the compound Y_9Co_7 which is the first very weak itinerant ferromagnetic superconductor. The results show the Curie temperature at about $T_C \approx 4.5K$ and the onset of superconductivity at about $T_{\approx}3.0K$, revealing the coexistence state of the superconductivity and ferromagnetism within some temperature interval below T_S. We focus attention on our recent magneto-resistance, magnetization and specific heat results for carefully-selected chemically-homogeneous polycrystalline specimen. A few of the old results on ultraviolet photoemission spectroscopy and band structure calculations are shortly reviewed and discussed. A set of normal state and superconducting quantities have been calculated within the Ginzburg- Landau- Abrikosov- Gorkov theory and have revealed the clean limit superconductivity of the compound.

Silicene – a silicon counterpart of graphene

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Silicene, a silicon equivalent of graphene, is a new two-dimensional material, one atom thick layer and made of silicon atoms. Despite its similarity in atomic and electronic structure to graphene, including the presence of highly mobile massless Dirac particles, silicene has some advantages that make it more useful from the point of view of applications in nanoelectronics. Not only is it compatible with current Si-based technology, but also its atomic and electronic structure is very sensitive to external influence.

In this talk a recent progress in fabrication and characterization of silicene will be discussed. A particular emphasis will be put on the problem of silicene interaction with a substrate. Furthermore, the methods of modification of the electronic structure, in particular allowing to control the width of the energy gap, will also be presented.

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Thermodynamics of simple cubic Hubbard model - dynamical mean-field study

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The Hubbard Hamiltonian is a canonical model for studying properties of correlated and itinerant electrons or cold fermionic atoms on lattices. Therefore, it is of great importance to obtain within a single method and collect in one place results on this model as a reference to other studies. Within the dynamical mean-field theory solved by the continuous time quantum Monte Carlo method, the program developed in our group, we provide a systematic and comprehensive solution of the Hubbard model in the infinite simple cubic lattice. Specifically, we study metal-insulator transition and thermodynamic properties such as internal energy, specific heat and double occupancy. After testing the new program we will solve the Hubbard model in the presence of different geometrical constrictions and inhomogeneities.

Properties of the fermion–phase model

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We use a hybrid approach that combines the exact diagonalization method with the Monte Carlo simulations to study the fermion-boson (FB) model. The FB model describes an exchange processes converting pairs of opposite–spin fermions into localized bosons (molecules or tightly bound local Cooper pairs) and vice versa. By replacing the boson operators with c-numbers we obtain an effective model in which fermions interact with classical phases (the *fermion-phase model*). The calculations show that the fermion-boson interaction leads to an effective long-range interaction between the boson phases which coherently order at low temperature and form vortex-antivortex pairs at higher temperature. We show that despite the presence of topological excitations there is no jump in the temperature dependence of the phase stiffness. This result suggests that there is no Kosterlitz-Thouless transition in the fermion-phase model. We propose a possible experimental realization of this model in a cold-atom system with fermionic atoms in two different hyperfine states loaded on an optical lattice.

Superconductivity with local electron pairing: BCS–BEC Crossover

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The crossover from a weak coupling BCS superconductivity of overlapping Cooper pairs to the Bose-Einstein condensation (BEC) of tightly bound preformed pairs has recently received great interest. We shall discuss basic concepts of the BCS-BEC crossover in Fermi systems and its possible realizations in condensed matter and ultra-cold fermionic atomic gases with tunable interactions. We review the evolution from the cooperative Cooper pairing (BCS superconductivity) to local pair formation and their (composite) boson superfluidity in systems with local attractive interactions. The models analyzed include: (i) the extended Hubbard model with on-site or intersite attractive interaction, (ii) the spin-imbalanced attractive Hubbard model and also the asymmetric (mass imbalanced) Hubbard model and (iii) the Boson-Fermion (BF) model with resonant interaction on a lattice. In particular, the superconducting characteristics of the BF model are determined as a function of position of the local pair level and total particle concentration, for different pairing symmetries on 2D square lattice. Moreover, the focus is on the superfluid transition temperature and phase diagrams of the BF resonant model for 3D (and quasi 2D) lattice, determined within the self-consistent T-matrix approach. The salient features of BCS-BEC crossover for various filling and across the superfluid-insulator transition in the BF model are analyzed. Our results are discussed in connection with a two-component scenario of preformed pairs and unpaired fermions for high temperature superconductors. They are also related to the superfluidity in ultra-cold fermionic atomic gases with a Feshbach resonance.

Relaxation in one– and two–dimensional spin systems.

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In a large number of generic many–body systems, it is conjectured that strong electronic correlations give rise to extremely fast times–scales of relevant relaxation processes. We study the relaxation mechanisms in Heisenberg and t-J models in one (1D) and two dimensions (2D). We show that relaxation of charge carriers in the 2D t-J model consists of two distinct stages. The initial ultrafast stage is based on generation of string states in the close proximity of the carrier. In the subsequent (much slower) stage local spin excitations are carried away by magnons. The relaxation time on the two-leg ladder system is an order of magnitude longer due to the lack of magnetic order. Finally, we discuss exotic properties of 1D spin systems, which relax (equilibrate) but may not thermalize.

Magnons

J. Morkowski

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Didactical lecture

Spin, momentum and chirality

M. Nowak

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I will review the consequences of Dirac equation, concentrating on exact and broken symmetries of the standard model.

Iron base superconductors – the problem of symmetry and pairing

Andrzej Ptok

Iron-base superconductors (FeSC) discovered in 2006, are multi-band layered materials, with characteristic Fermi surface. Questions raised about the type of pairing and symmetry existing in FeSC materials are still open.

In this lecture we show how to calculate the gap function in the fluctuation exchange (FLEX) approximation, to shed light on the nature of the superconducting state. We also discuss the role of the interband Cooper pair hopping interaction in FeSC.

This work has been partly supported by the National Science Center (NCN), through scheme MAESTRO, Grant No. DEC-2012/04/A/ST3/00342.

Magnetic properties of $(Ph_4P)_2[Mn(acacen)M(CN)_6]$ single chain magnets for M=Fe, Os, and M=Co

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Single chain magnet (SCM) behavior may be observed in crystals in which the exchange interaction between spins creates a quasi 1 dimensional system. Despite the lack of a long-range magnetic order at a finite temperature, SCMs may exhibit a remanent magnetization due to slow magnetic relaxation below a blocking temperature. As shown by Glauber in 1963, the relaxation time of ferromagnetically coupled chain of Ising spins follows the Arrhenius law with an activation energy barrier. The first experimental observation of such a behaviour was found 40 years later, and till today only few such examples exist.

During the talk I will present magnetic properties of the family of compounds built of Mn^{III} and Fe^{III} (or Os^{III}) ions linked into chains by cyanide bridges -CN-. These compounds appear to be very good SCMs. The parameters related to the SCM behaviour will be discussed basing on the experimental data analysis. This includes (1) the energy barrier of relaxation processes and their mechanism, (2) the easy axis magnetic anisotropy, (3) exchange interaction within the chains, (4) inter-chain interaction, (5) the influence of defects in the crystal structure.

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Superconductivity, charge density wave and magnetic order (spin density wave) in iron-based superconductors as seen by Mössbauer spectroscopy

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A review of the recent results obtained for the iron-based superconductors by means of the Mössbauer spectroscopy is to be given. In particular, the attention is to be focused on the interplay between various orders within these fascinating compounds. Namely, one encounters magnetic order in the form of the 3d spin density wave (SDW) being either longitudinal or in some cases transversal. This type of order is accompanied by the lowering of the crystal symmetry close to the magnetic transition. For some related compounds like FeAs or FeSb one observes SDW in the form of spirals and magnetic transition is accompanied by the lattice hardening. For compounds with transitions to the superconducting state there is neither 3d magnetic order nor lowering of the crystal symmetry. On the other hand, one sees (even at high temperature) development of the charge density wave (CDW) leading to the modulation of the electric field gradient (EFG) in the form of the EFG wave (EFGW). It is worth mentioning that 4f localized moments could order within superconducting phase in contrast to the 3d moments – the latter being absent within superconductor. The talk is to be focused on the ability of the Mössbauer spectroscopy to see the charge and/or spin (hyperfine field) modulation and the lattice hardening. *This work was supported by the National Science Center of Poland, DEC-2011/03/B/ST3/00446.*

Emergent Dirac fermions in graphene: Pseudospins, time-reversal symmetry, and quantum criticality

Adam Rycerz

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Graphene, together with other Dirac materials, represents a striking case of emergence in physics, as the system build of nonrelativistic components (such as carbon atoms at normal conditions) turns out to host relativistic quasiparticles. These quasiparticles show several unexpected features, such as additional quantum numbers (*pseudospins*) opening up new opportunities for quantum control in electronic devices [1], effective time-reversal symmetry which may be broken without magnetic fields [2], or *intrinsic* quantum criticality due to a peculiar band structure near the Fermi level [3]. Also, new macroscopic quantum effects have been recently demonstrated in condensed-matter Dirac systems [4]. In the talk, I will present a theorist's view on the topics listed above.

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Minimal conductivity and signatures of quantum criticality in ballistic graphene bilayer

G. Rut and A. Rycerz

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We study the ballistic conductivity of graphene bilayer in the presence of next-nearest neighbor hoppings between the layers. An undoped and unbiased system was found in Rut G. and Rycerz A., Phys. Rev. B, 89 (2014) 045421, to show a nonuniversal (length-dependent) conductivity $\sigma(L)$, approaching the value of $\sigma_\star = 3/\pi \simeq 0.95$ for large L. Here we demonstrate one-parameter scaling and determine the scaling function $\beta(\sigma) = \mathrm{d}\ln\sigma/\mathrm{d}\ln \mathrm{L}$. The scaling flow has an attractive fixed point ($\beta(\sigma_\star) = 0$, $\beta'(\sigma_\star) < 0$) reproducing the scenario predicted for random impurity scattering of Dirac fermions with Coulomb repulsion, albeit the system considered is perfectly ballistic and interactions are not taken into account.

Color superconductivity

M. Sadzikowski

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I discuss properties of hadronic matter at very high density and relatively low temperature. One expects that in this region of the QCD phase diagram a degenerate gas of quarks form a condensate of Cooper pairs at the Fermi surface. Therefore, a new phase of matter emerges which is called a color superconductor. In the first part of this review I encapsulate the most important features of Quantum Chromodynamics, including symmetry structure of the theory and its direct consequences. Subsequently, I present basic arguments which stand behind physical predictions connected to different kinds of color superconducting states. I discuss Color-Flavor-Locked (CFL) phase, 2SC phase and more complicated structures which can appear at moderate densities. In the last part, I show a possible connection between color superconducting phases and properties of compact stars.

Magnetism and superconductivity in strained and doped iron chalcogenides

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In Fe(Se,Te) systems an interplay between magnetism and superconductivity (SC) is complex and still intriguing. Interestingly, superconducting Fe(Se,Te) compounds exhibit spin fluctuations, originating from a single-stripe AFM order, connected with the (π, π) nesting. It is known that pure FeTe has a double-stripe antiferromagnetic (AFM) ground state and SC emerges under Se or S substitution into Te sites in bulk FeTe and also under tensile stress in FeTe thin films. Our first principles calculation (DFT) results indicate that, indeed, the single-stripe AFM order become a ground state of the superconducting films of tensile-strained FeTe [1]. Similarly, the partial substitution of FeTe with sulphur leads to the phase transition from double- to single-stripe AFM order. Since analogous phase transitions have been obtained also for hypothetical (Ru,Fe)Se and (Ru,Fe)Te systems, we postulate that they can be good candidates for new superconducting iron-based materials.

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Acknowledgments

This work was supported by the National Science Center of Poland under grants No. 2012/05/B/ST3/03095 and No. 2013/08/M/ST3/00927. Calculations were partially performed on ICM supercomputers of Warsaw University (Grant No. G46-13) and in Wroclaw Center for Networking and Supercomputing (Project No. 158).

Quantum oscillation studies of the Fermi surface of heavy fermion materials

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I will review quantum oscillation studies of heavy fermion materials and related compounds. These measurements give unique information regarding the full three-dimensional topology of the Fermi surfaces and the re-normalization of the quasi-particle masses. I will first briefly introduce the physics of heavy fermions and the concept of a quantum critical point. I will then discuss different types of quantum criticalities and associated changes of the Fermi surface. Next, I will discuss field-induced magnetic transitions in heavy fermions and the evolution of the Fermi surface across them. Finally, an essential issue in heavy fermion materials is the effect of magnetic field itself on the heavy quasi-particles. Theoretically, the effective masses of the spin-up and spin-down bands are predicted to be different and field-dependent. I will address this question from the experimental point of view. All the above will be illustrated by numerous examples of quantum oscillation experiments in Cerium-based heavy fermion compounds.

Correlated fermions in presence of spin-dependent disorder

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Inspired by recent development in experiments with cold atoms [1,2] we present theoretical results on correlated fermions on a lattice with spin-dependent disorder. In the first part we present the thermodynamical properties of the system away from half-filling, showing: magnetization, double occupancy and static susceptibilities [3]. Interestingly the spin-dependent disorder triggers the finite magnetization in the system. The second part is devoted to description of the system at half-filling and at T=0. The central result is the paramagnetic phase diagram showing the metallic, Mott insulating, and Anderson localized states.

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Unconventional superconductivity in t-J, Hubbard, and Anderson models: From spins to Cooper pairs

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We have formulated both the statistically consistent Gutzwiller approximation (SGA) [1], as well as the systematic diagrammatic expansion of the Gutzwiller wave function (DE-GWF) for both the Hubbard [2] and the t-J models [3]. The latter method leads to a proper doping independence of the Fermi velocity in the nodal direction. Both approaches provide a dome-like behavior of the superconductivity appearance in a semi-quantitative manner, as well as the doping dependence of extended the d-wave gap in the antinodal direction. The results coming from the models are critically overviewed [4].

The work was partly supported by the Project TEAM (from The Foundation for Polish Science) and Grant MAESTRO (from The National Science Centre), No. DEC-2012/04/A/ST3/00342.

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Phonons in $TaSe_2$ studied by ARPES and DFT calculations

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2H-$TaSe_2$ exhibits the transitions to incommensurate and commensurate charge density waves (CDW) at 122 K and 90 K, respectively. Its band structure was studied by ARPES at T=20 K. The obtained spectral functions show deviations from non-interacting dispersions near the Fermi energy, which reflect self-energy effects. We determined real ($Re\Sigma$) and imaginary ($Im\Sigma$) components of the self-energy as well as the effective electron-phonon coupling constants (λ_{el-ph}). Phonon spectrum in 2H-$TaSe_2$ was calculated by VASP and PHONON packages. Theoretical phonon density of states is compared to self-energies obtained from ARPES. Phonon softening is found at $\frac{2}{3}$ of the Γ-M distance what matches the CDW vector $q_{CDW} = \frac{1}{3}b^*$.

Topological phase diagram of $Pb_{1-x}Sn_xSe$

T. Story

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$Pb_{1-x}Sn_xSe$ IV-VI semiconductor is a topological crystalline insulator (TCI) - new 3D topological material exhibiting Dirac-like, helical surface states protected by crystalline symmetry. We applied angle- and spin-resolved photoemission technique to examine the topological transition to the TCI state for the (001) surface of bulk $Pb_{1-x}Sn_xSe$ monocrystals and the (111) surface of thin films. In the inverted band structure regime we found Dirac-like, in-gap spin-polarized states: close to four X-points for the (001) surface but at Γ- and three M-points for the (111) surface. Based on photoemission spectroscopic observations we construct the composition - temperature topological phase diagram of $Pb_{1-x}Sn_xSe$ and compare it with tight-binding band structure calculations.

Materials with correlated electrons; A pathway from Kondo insulator to superconductivity

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Strongly correlated f and d-electron systems are presently among the most intriguing and versatile materials, and their understanding represents one of challanges in condensed matter physics. A wide variety of interesting phenomena can be attributed to electronic correlations, among them metal-insulator transitions, heavy fermion and non-Fermi liquid behaviours, quantum criticality, and superconductivity. A key parameter in these materials is the exchange between local magnetic moments of the f-electron states and the conduction carriers, J_{sf}. As J_{sf} is changed, the system can be tuned from a magnetically ordered metal to a heavy Fermi liquid under change in temperature, alloy composition, field or pressure. This presentation will be a pathway from Kondo insulator to superconductivity. The topic of this report are Kondo insulators with narrow hybridization gap and the effects of metallization, and electronic structure, thermal and electric transport, and thermodynamic properties of skutterudite-related heavy fermions.

Coexistence of ferromagnetism and Kondo effect in f-electron intermetallic compounds

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I plan to review our recent works on the coexistence of ferromagnetism and Kondo effect in Np_2PdGa_3 [1], Np_2PtGa_3 [2] and $CePd_2P_2$ [3]. The intermetallic compounds were found to order ferromagnetically at 62.5 K, ~26 K and 28.4 K, respectively. I will show that the considered compounds share several common features: i) a competition of, at least, three different types of interactions—Kondo effect, Rudermann-Kittel-Kasuya-Yosida (RKKY), and crystal electric field (CEF) splitting, represented by an energy relationship $T_K < T_{RKKY} \sim \Delta_{CEF}$, ii) ferromagnetic Kondo lattice properties with a relatively high Curie temperature, enhanced effective masses and low charge carrier density. I will convince that the evolution of the magnetic ground states in the actinide compounds can be explained within the RKKY formalism and the coexistence of ferromagnetism and Kondo effect in these materials can be qualitatively understood in terms of the so-called $S = 1$ underscreened Magnetic Kondo lattice model, which has recently been developed by Perkins et al. [5] and Thomas et al [6]. Electronic properties of $CePd_2Pd_2$ will be compared to those of, e.g., CeNiSb, $CePd_2Ga_3$, $CeAgSb_2$, CeRuPO, previously reported in the literature.

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Spin transitor action driven by the helical magnetic field

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The spin transistor operation is based on the efficient control of the spin-polarized current. In majority of spin transistor designs, this control is realized with the use of the spin-orbit interaction. However, the spin transistors based on the spin-orbit interaction suffer from low signal levels resulting from low spin injection efficiency and fast decay of the spin states. Recently, an alternative design of the spin transistor has been proposed by Betthausen et. al. [Science 337 (2012) 324]. According to this porposal the spin control is performed using by the helical magnetic field. In the present work, we have simulated the spin transistor action in two-dimensional waveguides made of CdMnTe by the presence of spatially modulated magnetic field. We have shown that in the adiabatic regime the spin transistor action is obtained by the spin backscattering, which can be tuned by the Landau-Zener transitions. We have found that in the regime, in which the spin evolution is predominantly non-adiabatic, the additional dips appear in the transmission of electrons through the device. This effect have been explained in terms of resonant intersubband scattering between spatially modulated Zeeman-split energy bands. We have discussed the influence of this effect on the spin transistor operation.

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Intrinsic mechanism of dichroism in chiral multiband superconductors

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We shall present an analysis of the Hall conductivity $\sigma_{xy}(\omega, T)$ in time reversal symmetry breaking states of exotic superconductors. The intrinsic Kerr signal appears in a general multiband system. This is a novel mechanism which may explain the Kerr effect observed in strontium ruthenate and possibly other multiband superconductors. The proposed mechanism does not rely on impurity scattering or a finite width of the incident photon beam.

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

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Microscopic model for ferromagnetism in UGe_2

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Anderson lattice model is used to rationalize the principal features of the heavy fermion compound UGe_2 by means of the *generalized Gutzwiller approach* (the SGA method). This microscopic approach successfully reproduces magnetic and electronic properties of this material, in a qualitative agreement with experimental findings from the magnetization measurements, the neutron scattering, and the de Haas–van Alphen oscillations. Most importantly, it explains the appearance, sequence, character, and evolution in an applied magnetic field of the observed in UGe_2 ferro- and, para-magnetic phases as an effect of a competition between the f–f electrons Coulomb interaction energy and f–conduction electrons kinetic energy (hybridization).

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Beyond the standard Bose-Hubbard model description of cold bosons in optical lattices potential

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Examples of physics for bosons in optical lattices are considered which necessitate going beyond the standard Bose-Hubbard model. Such a situation appears typically for strong enough interactions. We discuss both the case of contact and dipolar interactions. For the former, an effective Hubbard-like single band model captures most of the physics. For dipolar interactions of moderate strength, the role of the so called density induced tunnelings (known as bond charge tunnelings in "condensed matter community") is shown to be of importance. Strong dipolar interactions make a standard tight binding expansion ineffective. Alternative approach which combines Wannier functions of lower bands with Bloch function representation of higher bands allows us to find quasi-stable configurations essentially equivalent to Majumdar-Ghosh states.

Unconventional superconductivity with interband pairing

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We analyze the general features of unconventional superconducting states with pairing between particles from the different bands. First, the so-called Hund's rule induced spin-triplet pairing is studied within the doubly degenerate Hubbard model by using the *Statistically consistent Gutzwiller Approximation*. It is shown that the correlation effect in conjunction with the Hund's rule lead to the stability of the paired phase in the purely repulsive interactions regime. It is also shown that the hybridization results in a Fermi wave-vector mismatch between the bonding and antibonding bands what has a destructive influence on the paired phase. Next, the idea of the spontaneous non-zero momentum pairing is introduced by using an exemplary four-band model with spin-singlet interband pairing, which refers to the two hole-like and two electron-like bands of an iron-based superconductor. It is shown that the Fermi wave-vector mismatch can be compensated by the nonzero momentum of the Cooper pairs what gives rise to the spontaneous FFLO type of phase.

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Posters

Effect of fluctuations of magnetization on bound magnetic-polaron state in ferromagnetic semiconductors

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We extend theory of the bound magnetic polaron (BMP) in diluted paramagnetic semiconductors to the situation with a ferromagnetic phase transition. This is achieved by including also the classical Gaussian fluctuations of magnetization coming from the quartic (non-Gaussian) term in the effective Ginzburg-Landau Hamiltonian for the spins. Within this approach, we find a ferromagnetically ordered state within the BMP in the temperature range well above the Curie temperature for the host magnetic semiconductor. Numerical results are compared directly with the recently available experimental data for the ferromagnetic semiconductor GdN. The agreement is excellent given the simplicity of our model and is due to the circumstance that the polaron size ($a_B \approx 1.4nm$) encompasses a relatively large but finite number ($N \approx 400$) of quasiclassical spins S = 7/2 coming from Gd^{3+} of BMP washes out the nation of critical temperature and thus makes the incorporation of classical Gaussian fluctuations sufficient to describes realistically the situation. ions. The presence of BMP washes out the nation of critical temperature and thus makes the incorporation of classical Gaussian fluctuations sufficient to describes realistically the situation.

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$(H_2)_n$ molecular system with ab-initio optimization of wave function in correlated state: computational implementation based on two-level parallelism.

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We analyze the $(H_2)_n$ molecular systems in the correlated state of 1s electrons. Our approach originates from variational, the so-called EDABI (Exact Diagonalization Ab Intitio Approach) method. The approach from consists of (*i*) construction of orthonormalized localized trial wave functions; (*ii*) microscopic parameters calculation; (*iii*) diagonalization, and (*iv*) variational optimization. For few molecule systems stage (*ii*) is computationaly most time-consuming and tractable efficiently in general case only if the Slater-type orbitals are represented by the Gaussian-type orbitals. We show how the combination of shared and distributed memory models can reduce the time of calculation by two orders of magnitude on modern HPC clusters where dozens of CPUs and hundreds of cores are simultaneously utilized. The natural way of parallelism application for a given context and some ground-state properties of the analyzed systems are discussed.

Acknowledgments. The authors are grateful to the Foundation for Polish Science (FNP) for support within the project TEAM, as well as to the National Science Center (NCN) through Grant MAESTRO, No. DEC-2012/04/A/ST3/00342. All the calculations were performed on the TERA HPC cluster belonging to the ACMiN, AGH University of Science and Technology, Krakow, Poland.

Electronic and transport properties of topological insulators

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We study the electronic and transport properties of various topological insulators. Topological insulators (TI) [1] are new materials, which posses many properties interesting for both applied and fundamental physics. In the following work, we analyze the Su-Schrieffer-Heeger model for polyacetylene [2] and CdTe/HgTe quantum wells in the Bernevig-Hughes-Zhang model [3]. The conductance and eigenenergy spectra are presented in case of a finite systems. We investigate the effect of various types of disorders and external potentials. The effect of magnetic field on CdTe/HgTe quantum wells will also be considered [4].

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Spin spirals in FeAs and FeSb studied by Mössbauer spectroscopy

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Iron pnictides compounds FeAs and FeSb were investigated by means of 57Fe Mössbauer spectroscopy versus temperature. The antiferromagnetic ordering temperature was found as 69 K for FeAs and 232 K for FeSb. The magnetic order leads to the incommensurate spin spirals propagating through the iron atoms in the direction of the c-axis with a complex pattern of the hyperfine magnetic fields distributed within a-b plane. Spiral symmetry corresponds approximately to the symmetry of the electron distribution within wave functions described by the angular momenta up to two, i.e. up to d electrons responsible for the itinerant magnetic order. Spin spirals are very similar in FeAs and FeSb despite different crystal symmetry, i.e. orthorhombic for FeAs and hexagonal for FeSb. The possible reason of this similarity is the octahedral coordination of iron by pnictogen.

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The correlation between the energy gap and the pseudogap temperature in cuprates: the YCBCZO and LSHCO case

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The paper analyzes the influence of the hole density, the out-of-plane or in-plane disorder, and the isotopic oxygen mass on the zero temperature energy gap ($2\Delta(0)$) for $Y_{1-x}Ca_xBa_2(Cu_{1-y}Zn_y)_3O_{7-\delta}$ (YCBCZO) and $La_{1.96-x}Sr_xHo_{0.04}CuO_4$ (LSHCO) superconductors. It has been found that the energy gap is visibly correlated with the value of the pseudogap temperature ($T^\star$). On the other hand, no correlation between $2\Delta(0)$ and the critical temperature (T_C) has been found. The above results mean that the value of the dimensionless ratio $2\Delta(0)/k_BT_C$ can vary very strongly together with the chemical composition, while the parameter $2\Delta(0)/k_BT^\star$ does not change significantly.

Relaxation times in semiconducting Dot Ring Nanostructures

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We study a nanostucture composed of a quantum dot surrounded by a quantum ring, named afterwards DRN (Dot-Ring Nanostructure), in a single-electron regime. We have already shown that many DRN's properties are strongly dependent on the distribution of the electron wave functions. Here we focus on the transport properties of the DNR coupled to two leads.

In the typical single electron transistor the switching characteristics is a results of the Coulomb blockade. Within our approach we propose to control the current by changing the strength of the coupling between the DRN and the electrodes. The idea is based on the fact that if the DRN's ground state is situated in the quantum dot part of the DRN, its overlap with wave functions of electrons in the electrodes is very small and so is the conductivity. On the other hand, if the DRN's ground state is in the ring part, it has a significant overlap with the electrodes' wave functions what results in a high conductivity. The ground state of the DRN can be moved with the help of an electrostatic gating. We also demonstrate that the DRN coupled in an asymmetric way to the source and drain electrodes can behave like a current rectifier.

Magnetism of $EuFe_2As_2$-based superconductors studied by ^{151}Eu and ^{57}Fe Mössbauer spectroscopy

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The $EuFe_2As_2$-based superconductors doped with Ca and Co were investigated by means of the ^{151}Eu and ^{57}Fe Mössbauer spectroscopy versus temperature. It was found that spin density wave (SDW) is suppressed by Ca and Co substitution i.e. a magnetic transition temperature is lowered together with the SDW amplitude. Iron spectra exhibit some non-magnetic component in the superconducting region, however traces of SDW survive in the region of superconductivity, so it seems that superconductivity has some filamentary character. Europium orders magnetically regardless of the Co and Ca substitution. Europium moments rotate from the a-axis in the direction of the c-axis (within a-c plane) with increasing amount of dopants. Iron experiences a transferred magnetic field from europium for the substituted material – in the SDW and non-magnetic states both. Europium magnetic order and superconductivity coexist in the same volume.

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Electronic properties of $CeNi_9In_2$ compound

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We studied a $CeNi_9In_2$ intermetallic compound, which is considered as a mixed valence (MV) system. Its electrical resistivity follows a Grüneisen - Bloch - Mott formula and is consistent with a Fermi liquid theory at low temperature. X-ray photoelectron spectra collected for Ce 3d level were analysed on the basis of Gunnarsson - Schönhammer theory. They yielded a parameter of the hybridization between f electrons and a valence band, which is Δ=104 meV. Ultraviolet photoemission spectroscopy was employed to study a valence band. Despite a high energy resolution a Kondo peak was not observed. Experimentally determined contribution from Ce 4f states is mainly located close to the Fermi energy (E_F). Peaks related to $f^1{}_{5/2}$ and $f^1{}_{7/2}$ final states are not resolved but form a broad peak or rather a plateau from 0.3 eV to E_F. Such f-electron density should correspond to a realization of MV state in $CeNi_9In_2$. The experimental data were compared to the calculations obtained with a full potential local orbital (FPLO) code.

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Space of symmetric functions in quantum Hall effect

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We consider elements of the ring of symmetric functions as candidates for wave functions in fractional quantum Hall effect (FQHE). It is known that so called Jack states are class of FQH states, with wave function given as a product of Gaussian function and Jack polynomial (boson state) or fermionic Jack polynomial (fermionic state). Laughin ($\nu = 1/r$), Moore-Read ($\nu = 2/(2m2)$, $m = 0, 1$ in the second LL), Read-Rezayi are Jack states.

In this poster we introduce Jack polynomials, present applications in FQHE and discuss properties. Moreover we introduce Macdonald polynomials - family of symmetric polynomials generalizing Jack polynomials, indexed by a partition of natural number and two parameters - t, q and present properties needed to construct fermionic Macdonald properties in basis of antisymmetric polynomials.

Spontaneous currents in bosonic rings

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Nonequilibrium dynamics of noninteracting bosons on a one-dimensional ring-shaped lattice is studied by means of the Kinetic Monte Carlo method. The system is approximated by the classical XY model (the kinetic term is neglected) and the Monte Carlo simulations are performed for the planar classical spins. We study the dynamics that follows a finite-time quench to zero temperature. In the quenching process the system has a disordered initial configuration corresponding to a high temperature and then the temperature drops to zero. If the quench is slow enough the system can equilibrate and finally reaches the ground state with uniform spin alignment at zero temperature. However, if the quench is faster than the relaxation rate, the system can get locked in a current-carrying metastable state characterized by a nonzero winding number. We study how the zero-temperature state depends on the quench. In particular, we find the average value of the current flowing in the zero-temperature state as a function of the quench rate.

Keywords: quantum ring, XY model, spontaneous currents

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Anisotropy of the gap parameter in the hole-doped cuprates: $YBa_2Cu_3O_{7-\delta}$

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The structure of the gap parameter ($\Delta_{\mathbf{k}}$) for the hole-doped cuprates has been studied. The obtained results indicate that the antinodal part of $\Delta_{\mathbf{k}}$ is very weak temperature dependent and above the critical temperature (T_C), it extends into the anomalous normal state to the pseudogap temperature. On the other hand, the values of $\Delta_{\mathbf{k}}$, which are close to the nodal part, are strongly temperature dependent. The model has been tested for the $YBa_2Cu_3O_{7-\delta}$ superconductor. It has been shown that the theoretical results agree with the experimental data.

FFLO state induced by the orbital effect in superconducting nanowires

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Unconventional superconductivity in the nanoscale regime has attracted growing interest due to the unique phenomena which appear if the electron motion is limited to the size smaller that the coherence length. In high-quality nanowires, the confinement of the electron transverse motion leads to the splitting of its energy band into the series of subbands participating in the superconducting state. Our results show that in the superconducting nanowires in the parallel magnetic field the FFLO state can be induced by the orbital effect. We have found that, at zero temperature, with increasing magnetic field a series of FFLO stability regions appear in between which the BCS superconductivity is stable. Our analysis shows that this effect is related to the non-zero momentum paring between electrons from different subbands.

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Theoretical studies of electronic properties of molybdenum disulfide nanostructures

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We study the electronic properties of MoS_2 nanostructures. Their honeycomb lattice, analogous to graphene, has importantly distinct properties to graphene. In MoS_2 monolayers the inversion symmetry breaking provokes valley-dependent optical selection rules for interband transitions at K points of hexagonal BZ. Moreover, we investigate spin-orbit coupling, which results in a large valence band spin splitting at the K point. The nanostructures studies include nanoribbons and quantum dots of various edge-types. We compare their properties to graphene structures of finite size. The electronic structure of quantum dots is obtained within the three-band TB model with the nearest-neighbours hopping included.

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An element specific look at the fate of Ce 4f spins in a heavy fermion surface intermetallic

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X-ray magnetic circular dichroism (XMCD) is a well established tool in magnetism research today. Being based on resonant absorption spectroscopy (XAS) at core thresholds, it is a sensitive probe of magnetic polarization of specific elemental and orbital character.

The talk shall present our recent efforts to gain insight into aspects of Kondo and Kondo lattice physics on the basis of spectroscopic characteristics and Ce 4f magnetic response with soft x-rays. The material of our choice is $CePt_5$, grown on single crystalline Pt(111). Its growth can be well controlled and the surface intermetallic thickness constitutes a remarkable tuning parameter for electronic structure and magnetic response alike. Based on our experiments we discuss (impurity) Kondo scale, screening of the Ce 4f moment and a number of possible signatures of lattice coherence that can be observed with this surface sensitive technique.

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Cover

front top: View from Przełęcz pod Kopą Kondracką (*Kopa Kondracka Pass*) by E. Kądzielawa-Major;
front bottom: Wielki Staw Polski (*Great Polish Pond*) by A. Kądzielawa;
back: Kozi Wierch (*Goat Peak*) by A. Kądzielawa;