0.1 Report on Workshop: "Magnetism, Superconductivity and Electron Correlations: celebrating the contributions and scientific legacy of Balázs L. Györffy"

H.H. Wills Laboratory, University of Bristol, Bristol (UK)

19.07.-21.07.2014

Psi-k Charity,
European Science Foundation (ESF), Centre Européen de Calcul Atomique et Moléculai (CECAM)-node Daresbury, University Bristol,
Leverhulme Trust

Organizers:
J.F. Annett, M. Gradhand, M. Lueders, J.B. Staunton

Given that the British summer was at its best from 19th to 21st July 2014, Bristol gave a splendid location for a scientific workshop with 54 international participants to celebrate the contributions and scientific legacy of Balázs L. Györffy". The scientific content of the workshop built upon the major working areas of the late Balázs L. Györffy: the cutting edge of fundamental condensed matter theory and material dependent predictions in the field of magnetism, superconductivity and alloy physics. This broad interest was well reflected by the talks which spread from as fundamental presentations as *"Density Functional Theory in the Absence of the Theorems of Hohenberg and Kohn: Constrained Search Formulation of the Theory"* by T. Gonis to the application of electronic structure theory to magnetism in realistic materials by M. C. Muñoz in *"Magnetism in oxide heterostructures: $LaAlO_3/SrTiO_3$"*. At the same time the audience heard historical overviews of his contributions in the field of superconductivity by D. A. Papaconstantopoulos and very recent results on the *"First-principles investigation of magnetism in lanthanide compounds"* exploiting the disordered local moment approach. Furthermore, current key questions were formulated such as *"Charge order in oxides: where is the charge?"* by W. E. Pickett and *"Magnetocrystalline anisotropy: How and from where does it arise?"* by O. Šipr. Recent and cutting edge results on the *"Laser-induced ultrafast demagnetization of ferromagnetic solids"* were presented by E. K. U. Gross and high trough put computational analysis for large classes of materials were discussed by G. M. Stocks in *"On the Physics of High Entropy Alloys - the Ultimate in Solid Solution Alloys"*. Finally, the scientific part of the workshop

was closed by an talk of J. Quintanilla who felt *"Haunted by Semiclassics"* after he was introduced to that topic by Balázs almost 15 years ago.

This and further presentations ranging from fundamental theory to material dependent description of various effects and mechanisms showed the full breadth of his work and opened the opportunity for stimulated discussions to all participants on a variety of aspects in condensed matter physics. Even though the British summer provided sun shine for the full three days the exchange of ideas during the extended lunch and coffee breaks often prohibited pleasant walks in the garden of Royal Fort House. Nevertheless, the participants enjoyed Bristol during the evenings after the conference reception on 19th and the poster session on 20th. The conference was concluded with a conference dinner in Goldney Hall Orangery where the warm sunny weather invited for walks in the surrounding gardens including discussions about very broad areas of modern physics.

The workshop was cosponsored by the Centre Européen de Calcul Atomique et Moléculaire (CECAM)-node Daresbury, the Leverhulme Trust, and the School of Physics and the Theory Group of the University of Bristol. We, the organizers and participants, would like to thank Psi-k and all other institutions for the support to this workshop.

Programme

	Day 1 (19.07.)	**Day 2 (20.07.)**	**Day 3 (21.07.)**
	Arrival		
8:30			
		Chair: G.M. Stocks	Chair: Q. Niu
9:00		M.A. Alam	W.E. Pickett
9:30		H. Ebert	P. Strange
10:00		C. Muñoz	M. Dennis
10:30		**Coffee**	
		Chair: P. Dederichs	Chair: P. Durham
11:00		G.M. Stocks	B. Újfalussy
11:30		O. Šipr	K.I. Wysokiński
12:00		**Lunch**	
		Chair: M.A. Alam	Chair: W.E. Pickett
14:00		A. Gonis	G.-Y. Guo
14:30		L. Szunyogh	D.A. Papaconstan-topoulos
15:00	**Registration**	Discussion	Discussion
16:00	**Coffee**	**Coffee**	
	Chair: R. Evans	Chair: A. Gonis	Chair: EKU Gross
16:30	E.K.U Gross	L. Petit	I. Mertig
17:00	Q. Niu	B. Klein	J. Quintanilla
17:30	**Welcome Reception**	**Poster Session**	
19:00			**Conference Dinner**

Abstracts

Compositional tuning of magnetic anisotropy of a Ni-based shape memory alloy

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The Ni-based Heusler alloy Ni_2MnGa is an interesting material with a large magnetic-field-induced-strain and magnetocaloric effect around TM, where TM is the structural cubic to tetragonal transition temperature. In the ferromagnetic tetragonal phase below TC, the alloy exhibits a magnetic shape memory effect which depends on its magnetic anisotropy.
We describe ab-initio DFT calculations of the effect and show how it can be increased when Fe is substituted for Mn which also acts to raise TC.

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Momentum space anisotropy of electronic correlations in Fe and Ni - an analysis of magnetic Compton profiles

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The total and magnetically resolved Compton profiles of Fe and Ni are computed using the Local Density Approximation of Density Functional Theory supplemented with electronic correlations treated at different levels. A rather good agreement between the measured and computed magnetic Compton profiles (MCPs) is obtained with the standard Local Spin Density Approximation (LSDA). By including local but dynamic many-body correlations captured by Dynamical Mean Field Theory (DMFT), the calculated magnetic Compton profile is further improved when compared with experiment. We discuss the range and capability of electronic correlations to modify the kinetic energy along specific spatial directions.

Giant Friedel Oscillations due to Quantum Well States in Thin Fe Films on W(001)

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Electrons mediate many of the interactions between atoms in a solid. Their propagation in a material determines its thermal, electrical, optical, magnetic and transport properties. Therefore, the constant energy contours characterizing the electrons, in particular the Fermi surface, have a prime impact on the behavior of materials. If anisotropic, the contours induce strong directional dependence at the nanoscale in the Friedel oscillations surrounding impurities. Here we report on giant anisotropic charge density oscillations focused along specific directions with strong spin-filtering after scattering at an oxygen impurity embedded in the surface of a ferromagnetic thin film of Fe grown on W(001). Utilizing density functional theory, we demonstrate that by changing the thickness of the Fe films, we control quantum well states confined to two dimensions that manifest as multiple flat energy contours, impinging and tuning the strength of the induced charge oscillations which allow to detect the oxygen impurity at large distances (≈50nm).

Vortices and spin-orbit effects in light and electron beams

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Electromagnetic radiation or electrons in the form of cylindrical wavepackets, or beams, carry orbital angular momentum and vortices along their axis. On account of the interplay between spin and orbital freedoms, however, such beams are not strictly eigenfunctions of L_z. Exact cylindrical solutions of Dirac particles can be written down, and the magnetic moment of the electron in this case follows directly from spin-orbit considerations [1]. In light beams, the axial vortices in such beams are a sensitive probe to scattering [2], and I will describe how after reflection, an order-ell vortex breaks up into a constellation of ell vortices whose configuration determines the high-order terms in the reflection (or more general scattering) operator [3].

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Orbital currents and orbital magnetism in magnetic solids

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The coherent treatment of spin and orbital currents provides the ultimate basis for a proper description of magnetic phenomena. In the first part of the talk a quantum-mechanical description of the magnetic shape anisotropy, that is usually ascribed to the classical magnetic dipole-dipole interaction, is presented [1]. This is achieved by including the Breit interaction, that can be seen as an electronic current-current interaction in addition to the conventional Coulomb interaction, within fully relativistic band structure calculations. The major sources of the magnetic anisotropy, spin-orbit coupling and the Breit interaction, are treated coherently this way. This seems to be especially important for layered systems for which often both sources contribute with opposite sign to the magnetic anisotropy energy. The second part of the talk deals with the definition for the orbital magnetisation of magnetic solids. Recent work on this issue makes use of a Bloch representation of the electronic structure [2]. Results for the spin-orbit induced magnetisation of Fe, Co and Ni based on this approach were presented by various authors [3]. To avoid the approximations and limitations of these investigations we present a coherent relativistic definition for the total magnetisation that is derived from the interaction of the total electronic current density with an external magnetic vector potential. Representing the electronic structure in terms of the Green function using the KKR band structure method leads to two terms that can be related to the Van Vleck and Landau contributions of the magnetic susceptibility [4]. A decomposition of the total magnetisation may be obtained by subtracting the spin part, that can be unambiguously determined, from the total magnetisation. Another route is to make use of the Gordon decomposition of the total electronic current density leading in a natural way to a spin and orbital contribution. Numerical results for the elemental ferromagnets Fe, Co and Ni will be presented and discussed.

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Stoichiometry, disorder and the Fermi surface of $MgCNi_3$

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Since the discovery of superconductivity with TC 7K [1], the antiperovskite $MgCNi_3$ has generated a great deal of excitement; the presence of superconductivity in such a Ni-rich compound has lead to speculation on the role of possible magnetic fluctuations, with experimental investigations [2] and band structure calculations suggesting that $MgCNi_3$ is close to a magnetic instability [3-5].
The debate about whether the superconductivity in $MgCNi_3$ is conventional is ongoing. Whilst early measurements on C-deficient polycrystalline samples were inconclusive [6], the recent advent of single crystals has allowed some clarification, with consensus tending towards medium to strong electron-phonon coupling as the dominant pairing mechanism [7]. However, the Ni deficiency of single crystals to date means that spin fluctuations may be reduced compared to the stoichiometric compound. This raises an important question: what effect does the Ni deficiency have upon the electronic structure?
Here, we present the bulk Fermi surface of $MgC_{0.93}Ni_{2.85}$ as inferred from high-resolution Compton scattering. We have performed complementary electronic structure calculations to study the effects of disorder introduced by Ni and C vacancies, through supercell calculations within the FP-APW+lo and pseudopotential formalisms. We have also treated the vacancy disorder within the coherent potential approximation in the KKR method.

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Sparsity of Superconductivity in Yb Heavy-Fermion Materials

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Superconductivity often emerges at the border of magnetism. This is well established and Ce based heavy fermion materials like $CeCu_2Si_2$ are prototypes of unconventional superconductivity arising at quantum critical points.
Heavy-fermion materials provide outstanding opportunities to study quantum critical phenomena including superconductivity as they can be tuned with control. The conventional order parameter description provides the framework to understand the critical fluctuations by mapping the problem to a classical phase transition with an increased effective dimensionality. These quantum critical fluctuations appear to be essential for emergent superconductivity. However, a growing number of materials require descriptions beyond the order parameter theory.
Remarkably, these unconventional materials lack superconductivity and many of them are Yb based heavy-fermion systems. Here, I will discuss signatures of unconventional quantum criticality in antiferromagnetic $YbRh_2Si_2$ and ferromagnetic $YbNi_4P_2$. The former is a well-studied prototype of unconventional quantum criticality with a Fermi surface reconstruction and energy-over-temperature scaling as inferred from Hall-effect measurements [1], indications for the violation of the Wiedeman-Franz law and unique behaviour of the Gruneisen parameter [2, 3].
The newly discovered ferromagnet $YbNi_4P_2$ also features unconventional behaviour of the Gruneisen parameter [4]. I present first electronic structure studies together with quantum oscillation measurements.

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Spin-flipping with conical magnets: Superconducting proximity effect in bi- and multilayers

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The interface between a superconductor and a ferromagnetic metal is the source of a variety of intriguing physical phenomena. Originating from the superconducting side of a bilayer system, spin-singlet Cooper pairs can penetrate the interface into the ferromagnetic side with the spin-singlet Cooper pair density showing a characteristic oscillating and decaying behaviour. However, if the interface allows for a spin-mixing effect, equal-spin spin-triplet Cooper pairs can be generated that can penetrate much further into the ferromagnetic side of the multilayer, known as the long-range proximity effect [1]. Here, we present results of spin-mixing based on self-consistent solutions of the microscopic Bogoliubov-de Gennes equations incorporating a tight-binding model. In a first part we interface a general conical magnet with an s-wave superconductor and analyse the influence of the conical magnetic angles on unequal-spin and equal-spin spin-triplet pairing correlations [2]. In a second part we include a specific conical magnet (Holmium) into our multilayer model to generate the spin-triplet Cooper pairs and analyse the influence of conical and ferromagnetic layer thickness on spin-triplet pairing correlations [3]. It will be shown that, in agreement with experimental observations [4], a minimum thickness of the conical magnet is necessary to generate a sufficient amount of equal-spin spin-triplet Cooper pairs allowing for the long-range proximity effect.
Balász L. Györffy was an inspiration in the original plan for this project, and he was a co-investigator on this EPSRC grant (EP/I037598/1). Sadly he passed away before the first results of this project were obtained.

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Band theory of the anomalous Hall effect in spintronic materials

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Anomalous Hall effect (AHE) refers to the transverse charge current in magnetic solids generated by an applied electric field. The AHE is an archetypal spin-related transport phenomenon and thus has received renewed interest recently, although discovered long ago in 1881 by Hall. In this talk, I will first give an introduction to band theoretical approaches to some issues in the field of AHE, especially, Berry phase theory and relativistic band structure methods for studying intrinsic Hall effects [1-3]. This will be followed by a review on our recent relativistic band theoretical studies on the AHE in isoelectronic L10 $FePd_{1-x}Pt_x$ alloys [4], Co-based Heusler compounds [5] and proximity-induced ferromagnetic Pt and Pd metals [6]. In particular, our theoretical calculations revealed that by increasing the Pt composition x, the intrinsic AHE in the $FePd_{1-x}Pt_x$ alloys can be significantly increased and that this chemical composition tuning of the AHE is afforded by the stronger spin-orbit coupling on the Pd/Pt site when the lighter Pd atoms are replaced by the heavier Pt atoms [4]. Furthermore, we predicted that the charge Hall current in Heusler compounds Co_2XZ (X=Cr and Mn; Z=Al, Si, Ga, Ge, In and Sn), except Co_2MnGa, would be almost fully spin polarized even though Co_2MnAl, Co_2MnGa, Co_2MnIn and Co_2MnSn do not have a half-metallic band structure. This suggests that these Heusler compounds have valuable applications in spintronics such as spin valves as well as magnetoresistive and spin-torque-driven nanodevices [5]. We will also show that significant anomalous Hall and Nernst conductivities can be found in nonmagnetic Pt and Pd metals [6], which exhibits a giant spin Hall effect [3], when placed next to a ferromagnet, thus lending support to the possible contamination of the pure spin current phenomena such as spin Seebeck effect measured by Pt.

The speaker thanks Shi-Ming Zhou, Jen-Chuan Tung, Tsung-Wei Chen, Qian Niu and Naoto Nagaosa for stimulating discussions and collaborations.

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Density Functional Theory in the Absence of the Theorems of Hohenberg and Kohn: Constrained Search Formulation of the Theory

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In 1964 Hohenberg and Kohn proved two remarkable theorems: First, they established a unique (within an additive constant) functional relation between a density, $n(\mathbf{r})$, that is known to describe the ground state of an interacting system of N particles under an external potential, $v(\mathbf{r})$, and the potential. Second, they demonstrated the existence of a density functional defined in terms of that potential whose minimum value is obtained for the density of the ground state of the system of interacting particles where it equals the energy of the interacting systems ground state. These theorems are considered to be the foundation of density functional theory (DFT). It is generally held that the density of the ground state of a potential, and only the density, suffices to determine the potential, the energy and the wave function of the ground state of an interacting many-particle system.

Unfortunately, however, given *only* the density, the methodology comprising density functional theory at present provides no procedure that determines the potential and the wave function of the ground state of a system, even if it is assumed that the density does describe the ground state of a potential. Most importantly, the theory cannot decide as to whether or not a given density corresponds to the ground state of a potential.

In this presentation, I show how the constrained search coupled with the process of differentiation with respect to the density determines whether or not a given density corresponds to the ground state of a potential, and if it does allows the unique determination (within a constant) of that potential as well as the ground state energy and wave function of an interacting many-particle system under that potential. These developments evolve from knowledge of the density alone with no reference to potential. In the new formulation, the theorems of Hohenberg and Kohn are replaced with generalized versions applicable to any density, a quantity that is the sole independent variable of the theory.

Computational results based on the new method are provided that demonstrate that the new approach solves rigorously the self-interaction problem, and establishes general conditions for the construction of a correlation energy functional.

Superconducting Materials: Competition Between Stability and High Tc

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Within the BCS theory of superconductivity the electron-phonon-interaction (epi) plays the role of binding mechanism for the Cooper pairs that condense to the superconducting state. The epi arises from the interplay of a lattice displacement and the perturbed response of the electron gas that leads to a change in the crystal potential and a renormalization of the bare phonons. In principle, increased epi leads to higher Tc without limit [1]. However, this qualitative argument for higher Tc can break down since a strong epi can also lead to dynamic instabilities in the underlying crystal structure and drive phase transitions that ameliorate the instability and degrade the potentially high Tc. We show several examples of this: carbonitrides [2] (e.g. NbC and MoN) and A15 materials [3] (e.g. V_3Si.) Particularly germane to this conference is the pioneering role that Balázs Györffy played in formulating a theory of the epi that enabled quantitative studies that elucidated the interplay between high Tc and lattice instabilities [4].

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Magnon Hall effect: A theoretical investigation

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Ferromagnetic insulators with Dzyaloshinskii - Moriya interaction show the magnon Hall effect (Y. Onose et al, Science 329 (2010) 297), i.e., a transverse heat current upon application of a temperature gradient. Our theoretical investigation is based on semiclassical transport theory, the Berry curvature and a quantum mechanical Heisenberg model. For two-dimensional Kagomé lattices, we establish a close connection of the magnon Hall effect with the topology of the magnon dispersion relation. From the calculated topological phase diagram, we predict a change of sign of the transverse thermal conductivity with temperature. The bulk-boundary correspondence is proven by topologically non-trivial edge magnons. Moreover, we provide a figure of merit for the transverse thermal conductivity and compare our results with experimental data for the pyrochlore system $Lu_2V_2O_7$.

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Magnetism in oxide heterostructures: $LaAlO_3/SrTiO_3$

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Complex transition metal oxides heterostructures (HS) have emerged as a powerful platform for engineering novel magnetic behavior in oxides. In fact, interfacial magnetism has been tailored in isolated interfaces and HSs of transition metal oxides. In addition, the two-dimensional electron gas (2DEG) formed at the (001) interface between two band insulators, $LaAlO_3$ and $SrTiO_3$, shows unusual magneto-transport properties. The existence of magnetism is perhaps one of the most surprising and least understood phenomena in this system. Based on first-principles density functional calculations we discuss the emergence of a magnetic state in the 2DEG formed in polar-oriented, $LaAlO_3/SrTiO_3$ HSs. We show that the electronic properties of the 2DEG are determined by the electronic structure of the $SrTiO_3$ and the crystallographic orientation of the interface. In both (001) and (111)-oriented $LaAlO_3/SrTiO_3$ HSs, the complex subband structure of the 2DEG promotes the development of a spin-polarized ground state. In the (001)-oriented HSs, the ferromagnetically coupled magnetic moments are mainly derived from the d_{xy} orbitals and mostly localized at the TiO_2 layer closest to the interface. Contrary, in (111) HSs the 2DEG is less confined, which allows to induce both, a metal-insulator and magnetic transitions by quantum confinement. We explore the possibility to design artificial magnetic phases by controlling the thicknesses of the STO layer.

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Geometric Phase Effects on Orbital Magnetism

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In this talk, I will review our semiclassical formula for orbital magnetization, which shows an important correction from the Berry curvature of the Bloch bands. The formula can be applied to metals as well as insulators, and is exact in the limit of zero magnetic field. I will also discuss our recent results on orbital magnetic susceptibility and electromagnetic polarizability, which requires a second order extension of our semiclassical theory for Bloch electrons.

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Applications of the Gaspari-Györffy Theory

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We first review applications of the Gaspari-Györffy theory which we performed over the years for a comprehensive list of single elements and compounds. We then present an application of the theory to pnictide superconductors and show that in the Fe-Se-Te system electron-phonon interaction is the possible mechanism.

First-principles investigation of magnetism in lanthanide compounds

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Using a combined density functional - disordered local moment approach [1, 2], we have investigated the magnetic ordering and critical temperatures of GdMg, GdZn, and GdCd. Excellent agreement with experiment is observed both at and away from equilibrium. In GdMg a transition from ferromagnetic to AF1 is observed with increasing pressure, whilst a canted magnetic state is seen to emerge from either the ferromagnetic or anti-ferromagnetic state with lowering the temperature. We find that despite being filled and situated at low binding energies, the non-lanthanide metal d-states strongly influence the electronic structure at the Fermi level and the magnetic ordering.

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Charge order in oxides: where is the charge?

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While the formal valence and charge state concepts have been, and remain, tremendously important in materials physics and chemistry, their very loose connection to actual charge leads to uncertainties in modelling behaviour and interpreting data and, not least, in actually understanding the microscopic processes that drive the transitions. We point out, selecting from several examples of transition metal oxides that we have studied (La_2VCuO_6, $YNiO_3$, $CaFeO_3$, $AgNiO_2$, V_4O_7, and the peculiar vegetable AgO) that while dividing the crystal charge into atomic contributions is indeed an ill-posed activity, the *3d occupation* of a cation [1] (and more particularly, differences in occupation) is readily available from first principles calculations. We discuss some examples, which include distinct charge states and charge-order (or disproportionation) systems, where different "charge states" of cations have *identical 3d* orbital occupation. Implications for theoretical modeling of such charge states and charge-ordering mechanisms will be discussed.
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Haunted by Semiclassics: from optical lattices through muonium to magnetic monopoles

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One of Balazs Györffy's latter scientific loves was semiclassics [1,2]. As a PhD student in Bristol (1997-2001) I was exposed to this point of view and I was supposed to have been exploiting it in my research. I didn't, though, and as a result I've been haunted by semiclassics ever since. For this I consider myself very fortunate. I will describe how, later on, a semiclassical approach allowed me and Chris Hooley to understand a crucial feature of optical lattices [3]; relate a personal anecdote involving muonium were semiclassics also played a key role [4]; and, finally, present a new, semiclassical theory [5] predicting bound states between artifical monopoles and 2D electrons a new twist on a century-old problem initiated by Poincaré [6].

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Magnetocrystalline anisotropy: How and from where does it arise?

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Magnetocrystalline anisotropy is one the of the key properties that determine the practical applicability of systems with magnetic atoms and clusters. To get a full picture, one needs not only to calculate the magnetocrystalline anisotropy energy (MAE) as accurately as possible but also to understand intuitively which factors affect it in various ways.

An intuitively appealing question in connection with the MAE of adatoms and films is whether the MAE comes only from the magnetic adatoms or whether there is also a sizeable contribution from the substrate [1]. In principle, the question about the localization of the MAE cannot be answered because energy is not an extensive quantity. However, by a careful choice of model systems where the spin-orbit coupling and the exchange field are selectively switched on and off, one can still get a well-defined insight into how different atoms contribute. This approach is illustrated by inspecting the MAE for Co adatoms and monolayers on Pd, Pt, Cu, Ag, and Au surfaces [2].

Another interesting problem is what is the physical cause for the MAE. Even though it has been known for decades that the MAE is linked to the spin orbit coupling (SOC), the specific mechanism how does it arise for concrete systems is still subject to debate. It will be demonstrated that for 3d transition metal adatoms on Au(111) the MAE can be linked to SOC-induced changes in the orbitally-resolved density of states upon the rotation of the magnetization. As a result of this, the MAE crucially depends on the position of the Fermi level of the substrate with respect to the energy bands of the adatom.

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On the Physics of High Entropy Alloys the Ultimate in Solid Solution Alloys

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The development of metallic alloys is arguably one of the oldest of sciences, dating back at least 3,000 years. It is therefore very surprising when a new class of metallic alloys is discovered. High Entropy Alloys (HEA) appear to be such a class and, as a consequence, one that is receiving a great deal of attention in terms of the underlying physics responsible for their formation as well as combinations of properties that make them candidates for technological applications. The term HEA typically refers to alloys that are comprised of 5, 6, 7 elements at or near equi-atomic composition that form random solid solution alloys on simple underlying lattices; FCC $Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2}$ [1] and BCC $Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2}$ [2] being textbook examples. The appellation High Entropy Alloy refers to an early conjecture [3] that these unusual systems are stabilized as solid solutions by the high entropy of mixing associated with the large number of components. Here, I will discuss two sets of questions posed by these systems. Firstly, how do we predict which combinations of N elements from the periodic table are most likely to yield a single phase solid solution HEA? Secondly, for systems comprised of the magnetic 3d-transition metals elements, what is the range of magnetic properties that particular HEAs are likely to exhibit? In both cases, I will present answers to some of these questions while emphasizing the need to address many others. For the former, I will propose a model that, through the use of high throughput computation of the enthalpies of formation of binary compounds, predicts the specific multi-elemental combinations most likely to form single-phase HEAs. For the latter, I will present the results of KKR-CPA and Monte-Carlo simulations of the finite temperature magnetic properties that point to the wide range of magnetic properties that one can expect from different elemental combinations, ranging from robust ferromagnetism to spin-glass like behavior.

This work was performed in collaboration with M. Claudia Troparevsky, James R. Morris, Andrew R. Lupini, Paul R. C. Kent, Markus Daene, Markus Eisenbach, Junqi Yin and Khorgolkhuu Odbadrakh and is supported by the Materials Sciences and Engineering Division of the Office of Basic Energy Sciences US-DOE.

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The Dirac Oscillator: Theory and Applications

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The Dirac oscillator is a simple exactly soluble model within relativistic quantum mechanics [1]. In this talk we introduce and discuss the standard theory of the Dirac oscillator. We then go on to show that it is equivalent to the Jaynes-Cummings Hamiltonian from quantum optics [2] and can also be transformed into a model which describes the properties of some two-dimensional materials [3]. Finally we discuss a chiral phase-transition that the Dirac oscillator undergoes in a magnetic field [4] and suggest experiments to observe it.

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Magnetism of itinerant electrons: good moments versus induced moments

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The framework of Disordered Local Moments (DLM) as introduced by Balazs Györffy and co-workers almost 30 years ago [1] provides a sensible ab initio theory of itinerant electron magnetism. We briefly summarize the progress of the DLM theory made during the past three decades. In particular, we focus on the relativistic [2] and finite temperature extensions [3,4,5] of the DLM scheme and discuss how the concept of good and induced moments is captured by the theory.

Related to real-time spin-dynamics we also highlight the possibility to calculate spin-model parameters from DLM [6,7]. Current problems how to include (i) induced moments into spin-models and (ii) the temperature dependence of the spin-model parameters will be discussed.

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Ligand design for long-range magnetic order in metal-organic frameworks

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The control of magnetic interactions in the metal-organic frameworks has yet to be proved, with current system displaying critical temperature of less than 10 K. We demonstrate computational chemistry can be used to predict and design material with desired properties. Using the Goodenough rules a new class of coordination polymer with long super-exchange interaction has been designed. Density functional calculations have been performed to calculate the magnetic properties of them. A Néel temperature above liquid nitrogen, as well as an extraordinary distance between the two metal centres, is predicted for such compounds. This model opens a new perspective in the development of magnetic metal organic frameworks.

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Monopole Hopping and Quantum Spin Tunnelling in Spin Ice

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The low temperature dynamics in spin ice materials is governed by the density and mobility of elementary excitations that behave as emergent magnetic monopoles. The diffusion of such monopoles proceeds via flipping of large electronic spins with Ising-like anisotropy (due to their crystal field environment). Experimental evidence suggests that, at temperatures relevant for spin ice physics, this flipping occurs as a quantum-mechanical tunnelling through a large anisotropy barrier. Here we investigate this process at the microscopic, single-ion level by computing the quantum dynamics resulting from the interplay between the crystal field Hamiltonian and the Zeeman coupling with magnetic fields (either applied or due to other spins). We interpret our results in terms of monopole hopping rates, and we compare our predictions with existing experiments for both $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$.

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The Kerr effect and dichroic sum rule in chiral superconductor

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The complex character of the superconducting order parameter can break time reversal symmetry, which gives rise to a non-vanishing contribution to the optical conductivity $\sigma_{xy}(\omega, T)$ of Sr_2RuO_4 in the absence of external magnetic field. This is measure by the optical Kerr effect appearing in a superconducting state. Theoretically in one band superconductors non-zero contributions to the Hall effect can arise from collective modes outside particle-hole symmetric point or from impurity scattering of quasiparticles. However, it was shown that in multi band superconductors an intrinsic contribution is possible [1,2] which is by construction zero in the one band case. Interestingly the effect sets in at the threshold frequency of the order of interorbital hybridization t' [2,3,4] and not at the expected frequencies of the order of 2Δ, where Δ is the magnitude of the order parameter. At the heart of the effect is the special form of the order parameter having C2 symmetry in alternating orbitals of the xz and yz character. These are the same orbitals which contribute to the orbital moment of the condensate calculated earlier [5]. In the talk the analysis of the dichroic sum rule relating the integrated Hall spectrum to the orbital moment will be discussed [1].

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