HCM Newsletter

Ψ_k Network

AB INITIO (FROM ELECTRONIC STRUCTURE) CALCULATION OF COMPLEX PROCESSES IN MATERIALS

Number 9 June 1995

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Editorial

In this Newsletter, as usually, the abstracts are placed at the end, before the **Highlight of the Month Section**. This section contains an article by **Lifshitz and Kosevich**, of interest to the *'magneto-oscillatory coupling community'*. It appears here owing to the translation from Russian by *Ivonna Siraskova* (Brno), and due to the work, interest and dedication of *Balazs Ujfalussy* (Budapest and Vienna).

In the section **News from the Network** we have repeated the steps which need to be followed when one wants to make a collaborative visit within the Network. Moreover, we repeat the formula to be used for acknowledging the Network.

In the section **News from the Working Groups** you will find reports on collaborative visits and/or workshops. Straight after the reports you can find **announcements of a postdoctoral position in Washington, D.C., and a Ph. D position in Munich.**

The *Network* has a home page on World Wide Web (WWW). Its *Uniform Resource Locator* (URL) is:
http://www.dl.ac.uk/TCSC/HCM/PSIK/main.html

This also contains pointers to several other nodes: *O.K. Andersen (Stuttgart)* which includes information on the **Network Conference**, *B.L. Gyorffy (Bristol)*, *J. Nørskov (Lyngby)* with information on CAMP, *M. Scheffler (FHI Berlin)*, and *A. Walker (UEA Norwich).* If you maintain a home page on your activities we will be happy to include a pointer from the *Network's* home page to your home page.

Please submit all material for the next newsletters to the email address below.

The following email addresses are repeated for your convenience, and are the easiest way to contact us.

	function
psik-coord@daresbury.ac.uk	**messages to the coordinator & newsletter**
psik-management@daresbury.ac.uk	**messages to the NMB**
psik-network@daresbury.ac.uk	**messages to the whole Network**

Dzidka Szotek & Walter Temmerman
e-mail: psik-coord@daresbury.ac.uk

News from the Network

Network's Policy for Collaborative Visits

With respect to collaborative visits and workshops organised by the Network, the agreed policy is to cover travel costs and provide per diem of 40 ECU, which in justified circumstances can be increased.
Since the procedure of applying for financial support for collaborative visits within the Network appears not to be entirely clear, we would like to repeat the necessary steps that it involves.

- One should submit a short (at most a page) proposal, detailing the scientific content of the proposed visit together with the planned duration and cost of one's visit, to **psik-management@dl.ac.uk**. If the standard per diem of 40 ECU would not be sufficient to cover the essential living and accomodation expenses, one should also provide the reasons and an estimate of the actual costs.
- If within one week there will be no objection to the proposed visit by any member of the Network's Management Board, one should consider one's visit approved.
- After the visit one should submit a report on the visit to **psik-coord@dl.ac.uk**, to be published in the next Newsletter, and a claim form for one's expenses with attached tickets. The claim forms can be obtain from us by sending e-mail to **psik-coord@dl.ac.uk**.
- One should acknowledge the Network in all publications that have resulted from collaborations and/or owing to a computer code obtained from the visited node, or at any of the 'hands-on computer codes' workshops organised by the Network. Also, one should send a copy of such publications to **psik-coord@dl.ac.uk**.

The following formula could be used in the acknowledgement:

This work has benefited from collaborations within, and has been partially funded by, the Network on "Ab-initio (from electronic structure) calculation of complex processes in materials" (contract: ERBCHRXCT930369).

If the Network's funds have not actually been used, but the work has benefited from some form of collaboration or a computer code distributed within the Network, then the part of the sentence: *...", and was partially funded by," ...* should be omitted in the above acknowledgement.

News from the Working Groups

Report on:

SPIN-ORBIT INFLUENCED SPECTROSCOPIES OF MAGNETIC SOLIDS

a workshop funded by the ESF - network:

RELATIVISTIC EFFECTS IN HEAVY ELEMENT CHEMISTRY AND PHYSICS

(coord.: P. Pyykkö, Helsinki and B. Hess, Bonn)

and the EU-HCM - network:

AB INITIO (FROM ELECTRONIC STRUCTURE)
CALCULATION OF COMPLEX PROCESSES IN MATERIALS

(coord.: W.M. Temmerman, Daresbury)

at Herrsching (D), from 20^{th} - 23^{rd} April 1995

organized by H. Ebert and G. Schütz

The aim of the workshop was to bring together researchers from all over Europe, active in the field of **Spin-orbit influenced spectroscopies of magnetic solids** and related topics, to present and discuss their latest results and ideas.

Due to the fact that about half of the funding for the workshop was supplied by the ESF-network on "*RELATIVISTIC EFFECTS IN HEAVY ELEMENT CHEMISTRY AND PHYSICS*" (REHE) (the other half was provided by the HCM-network coordinated by W. M. Temmerman), it was possible to bring together not only theorists from the HCM-network on "AB INITIO (FROM ELECTRONIC STRUCTURE) CALCULATION OF COMPLEX PROCESSES IN MATERIALS" but also theorists from outside this network as well as many experimentalists. Furthermore, it should be mentioned that nearly all groups organized in the EU-HCM-network on "*NOVEL PROBES FOR MAGNETIC MATERIALS AND MAGNETIC PHENOMENA: LINEAR AND CIRCULAR X-RAY DICHROISM*" were also represented. The ratio between theorists and experimentalists was about 1:1, resulting in very fruitful discussions after the talks but also during coffee breaks and in the evening in the so-called *Magnetic Bierstube*.

Consistently with the title of the workshop various contributions (see programme and abstracts below) reflected many different possibilities in which the spin-orbit interaction can influence the spectroscopical properties of magnetic solids - just giving rise to some additional structure in the spectra or to phenomena not present in paramagnets. The magneto-optical Kerr-effect, - a classical example for this was addressed by J. Kübler, P. Oppeneer, D. Weller, and - in its non-linear form - by W. Hübner. Relativistic effects and magnetic dichroism in photoemission for valence (J. Braun, A. Rampe) as well as core electrons (U. Hillebrecht, G. van der Laan) were discussed. A theory to describe the Auger-spectroscopy of magnetic systems was presented by P. Weinberger. Most contributions (talks by D. Arvanitis, M. S. S. Brooks, K. Capelle, P. Carra, C. T. Chen, H. Ebert, A. Fontaine, G.-Y. Guo, H. König, G. Krill, G. Sawatzky, J. Stöhr, P. Strange, as well as posters by D. Schmitz and J. Schwitalla) were related to magnetic dichroism in X-ray absorption (XAS). The main issue of these talks was the validity and applicability of the sum rules to deduce spin- and orbital magnetic moments from experimental spectra. For this reason the contributions of M. S. S. Brooks, B. Johansson, and L. Szunyogh on the importance of the spin-orbit coupling and the orbital polarisation mechanism for these moments perfectly fitted into the programme. XAS at high energies i.e. magnetic EXAFS and the interpretation of the corresponding spectra were addressed by C. Brouder and G. Schütz. The inverted XAS i.e. magnetic dichroism in fluorescence was the topic of B. Gyorffy's talk. Applications of the magnetic dichroism in XAS to investigate magnetic coupling and domain structures were presented by C. T. Chen and C. M. Schneider. M. J. Cooper's and K. Baberschke's talks on Compton scattering and ferromagnetic resonance, respectively, demonstrated that XAS is not the one and only tool to get information on spin- and orbital magnetism. A scheme to treat the relativistic effects in an approximate way and its application to scattering at free atoms was presented by L. Fritsche. Finally, P. Pyykkö reminded us that spin-orbit coupling has its impact not only on electron spectroscopies but also for example in nuclear quadrupole resonance spectroscopy.

(Hubert Ebert and Gisela Schütz)

Programme

Friday, April 21.

J. Kübler, Darmstadt
Calculated magneto-optical properties of transition metals and their compounds

D. Weller, San Jose
Magneto Optical Spectroscopy in strongly anisotropic systems: FePt and Co

M. S. S. Brooks, Karlsruhe
Relativistic Effects in Actinides

P. M. Oppeneer, Dresden
Spin-orbit transmission effects in the Kerr spectra of compounds: an ab initio study

W. Hübner, Berlin
Nonlinear Magneto-Optical Response of Thin Ferromagnetic Films

G. Sawatzky, Groningen
Magnetic X-Ray dichroism in studies of both short and long range magnetic order in antiferromagnetica

G. Krill, Orsay
Magnetic Circular X-ray Dichroism in RE/TM intermetallic compounds Role of the hybridization between 4f and the conduction electrons

G.-Y. Guo, Daresbury
Band Theoretical Investigation of Circular Magnetic X-ray Dichroism Sum Rules for Magnetic Multilayers

D. Arvanitis, Uppsala
An angle dependent MCXD study of Ni, Co and Fe on Cu(100); Experiment versus Theory

M. J. Cooper, Warwick
Spin and orbital moments in rare earth ferromagnetic compounds studied by Compton scattering

B. L. Gyorffy, Bristol
Dichroism in X-ray Fluorescence

B. Johansson, Uppsala
Enhancement of orbital magnetic moments at surfaces

C. Brouder, Paris
Multiple-scattering approach to magnetic EXAFS

Saturday, April 22.

P. Weinberger, Wien
Relativistic AES

U. Hillebrecht, Düsseldorf
Angular dependent magnetic dichroism in core level photoemission

G. van der Laan, Daresbury
Magnetic Ground State Properties and Angular Dependent Magnetic Dichroism in Core Level Photoemission

A. Rampe, Aachen
Linear magnetic dichroism in the angular distribution of photoelectrons (LMDAD) from the valence bands of Co(0001) and Fe(110)

G. Schütz, Augsburg
Magnetic EXAFS

P. Carra, Grenoble
Unified approach to near-edge X-ray phenomena

C. T. Chen, Murray Hill
Orbital and spin magnetic moments from soft-X-ray MCD

A. Fontaine, Orsay

Spin polarization of conduction electrons in metallic multilayers and intermetallic compounds from X-ray magnetic circular dichroism

J. Stöhr, San Jose
Angle-Dependent XMCD - Probing the Microscopic Origin of Magnetic Anisotropy

H. Ebert, München
Multiple scattering approach to magnetic dichroism in electron spectroscopy of transition metal systems

K. Baberschke, Berlin
Ni and Co single layers: Thickness dependence of Tc, the magnetic moment and the anisotropy

L. Szunyogh Relativistic study of magnetism of 4d, 5d transition metal overlayers on Ag(001) and Au (001)

C. M. Schneider, Berlin
Imaging of magnetic domains by means of magnetic dichroisms: magnetic spectro-microscopy

Sunday, April 23.

K. Capelle, Würzburg
Off-Diagonal Spin-Orbit Coupling in Superconductors

H. König, Grenoble
X-ray Absorption in a Tight-binding Band Structure Approach

P. Strange, Keele
On the Interpretation of MXCD Experiments on Itinerant Magnets

L. Fritsche, Clausthal-Zellerfeld
Treating Electronic excitations in Magnetic Materials by Solving Fully Relativistic Two-Component One-Particle Equations

J. Braun, Osnabrück
Relativistic effects in inverse photoemission

P. Pyykkö, Helsinki
Relativistic effects on nuclear quadupole coupling

List of Participants

D. Arvanitis (Uppsala), M. Battocletti (München), K. Baberschke (Berlin),
G. Bauer (Delft), J. Braun (Osnabrück), M. S. S. Brooks (Karlsruhe),
C. Brouder (Paris), K. Capelle (Würzburg), P. Carra (Grenoble),
C. T. Chen (Murray Hill), M. J. Cooper (Warwick), P. H. Dederichs (Jülich),
M. Deng (München), C. Demangeat (Strasbourg), H. A. Dürr (Daresbury),

H. Ebert (München), R. Feder (Duisburg), L. Fritsche (Clausthal),
H. Freyer (München), A. Fontaine (Orsay), J. Goedkoop (Grenoble),
G. Güntherodt (Aachen), G.-Y. Guo (Daresbury), B. L. Gyorffy (Bristol),
U. Hillebrecht (Düsseldorf), D. Hartmann (Aachen), W. Hübner (Berlin),
B. Johansson (Uppsala), G. Kaindl (Berlin), P. Kienle (München),
E. Kisker (Düsseldorf), M. Knecht (München), H. König (Grenoble),
G. Krill (Orsay), J. Kübler (Darmstadt), M. Mikami (Yokohama),
P. M. Oppeneer (Dresden), P. Pyykkö (Helsinki), A. Rampe (Aachen),
G. Sawatzky (Groningen), D. Schmitz (Jülich), C. M. Schneider (Berlin),
G. Schütz (Augsburg), J. Schwitalla (München), J. Stöhr (San Jose),
P. Strange (Keele), Z. Szotek (Daresbury), L. Szunyogh (Budapest),
W. M. Temmerman (Daresbury), G. van der Laan (Daresbury),
A. Vernes (München), P. Weinberger (Wien), W. Weber (München),
D. Weller (San Jose)

A list of the addresses of the participants is available upon request (email) from H. Ebert.

Abstracts

An angle dependent MCXD study of Ni, Co and Fe on Cu(100); Experiment versus Theory

J. Hunter Dunn[1], **D. Arvanitis**[1], N. Mårtensson[1],
M. Tischer[2], F. May[2], M. Russo[2], K. Baberschke[2]
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[2]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Germany

We report MCXD measurements of Ni, Co and Fe overlayers on a Cu(100) surface. The samples were prepared and characterized in situ, in ultra high vacuum. Out of plane elliptical X-ray light was used from a bending magnet at the storage ring BESSY in combination to an SX 700 plane grating monochromator. Data were collected around the overlayer $L_{3,2}$ edges. MCXD measurements as a function of the X-ray incidence angle for thicker overlayers show that saturation effects clearly modify the intensity distribution of the $L_{3,2}$ peak heights for the grazing X-ray incidence angles. This effect is therefore particularly important in the case where the magnetization easy axis is parallel to the surface. We have taken saturation effects into account before deriving information on magnetic moments using MCXD sum rules. By applying the sum rules to thick overlayers we find values for the magnetic moments that differ from the known ground state ones [1]. Possible reasons for this discrepancy will be discussed. One such contribution to the MCXD signal, is the existence of final states of s character. We present experiments of controlled oxygen contamination in the case of Ni overlayers on Cu(100) that allow one

to quantify experimentally the MCXD contribution of these states. These experiments also yield information on the influence of light contaminants on the magnetic properties of metal overlayers.

[1] J. Hunter Dunn, D. Arvanitis, N. Mårtensson, M. Tischer, F. May, M. Russo, K. Baberschke, J. Phys. C **7**, 1111(1995)

Ni and Co single layers: Thickness dependence of Tc, the magnetic moment and the anisotropy

Baberschke[1], M. Tischer, B. Schulz, A. Aspelmeier, M. Farle, D. Arvanitis
[1] Inst. für Atom- und Festkörperphysik (WE 1), Freie Universität Berlin, Arnimallee 14, D-14195 Berlin - Dahlem

MCXD /1/, ferromagnetic resonance /2/, and susceptibility /3/ measurements are reported for Ni and Co single layers mostly on Cu(100). Emphasis is given to the full thickness dependence of Tc and the critical exponent beta and in addition to the temperature dependence of M(T) and the anisotropy energy K(T). It appears to be important to analyze K as function of the reduced temperature t = T/Tc. The "surface" contribution of K is separated and the origin of a crossover between in- and out-of-plane will be discussed.

In the ultrathin limit an enhancement of the ratio orbital/spin moment is measured for Co/Cu(100) and a reduction of the total moment can be seen for Ni/Cu(100). For the later case the anisotropy of the magnetic moment can also be seen.

/1/ M. Tischer et al. Surf. Sc. 307, 1096 ('94)
/2/ B. Schulz et al. Phys. Rev. B50, 13467 ('94)
/3/ M. Tischer et al. J. MMM 135, L1 ('94)

Relativistic effects in inverse photoemission

J. Braun
Universität Osnabrück

The relativistic one-step theory is applied to inverse photoemission from the Ir(111)-surface. In the framework of a completely new developed surface contribution theoretical spectra are compared with corresponding experimental data. Herein the matrix elements for the surface contribution have been calculated in considering the image-potential behaviour of the barrier. Furthermore, it will be shown that relativistic effects induced by the bulk crystal modify the calculated spectra.

Relativistic Effects in Actinides

M.S.S. Brooks[1], A. Delin[2], O. Eriksson[2] and B. Johansson[2]
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[2] Condensed Matter Theory Group, Institute of Physics,
University of Uppsala, BOX 530, S-75121, Uppsala, Sweden

The effect of spin-orbit coupling upon the calculated pressure-volume relationship and upon the magnetic equation of state is summarized.

The local, diffuse and orbital magnetization and moment densities of 3d transition metals and actinides are compared. In the actinides the diffuse moments (mostly 6d in character) are anti-parallel to the local spin moments (mostly of 5f character) whereas the orbital moments (mostly of 5f character) are anti-parallel to the local spin moments and very large. Neutron diffraction results are analysed and comparison with theory yields the ground state spatial local, diffuse and orbital ground state magnetization densities. In particular the large orbital moments in actinides have been both measured and calculated from first principles.

Initial results for M4 and M5 edge magnetic circular dichroism in actinides selects primarily the 5f orbital moment, resolved in energy. Calculations of the magneto-optical Kerr effect for the actinide compound US, while agreeing with measurements in the 2eV range, produce a peak at 4eV which is not observed.

Spin-Orbit Effects in Superconductors with Heavy Elements

Klaus Capelle
Institut für Theoretische Physik, Universität Würzburg

Starting from a recently proposed relativistic theory of superconductivity, the counterparts of the Dirac equation and the Pauli equation are derived for superconductors. In the non-relativistic limit the conventional theory of superconductivity is regained. Up to order $(v/c)^2$ one obtains, besides the usual Darwin, spin-orbit and kinetic energy corrections, new off-diagonal spin-orbit and Darwin terms involving the pair potential in place of the electrostatic potential. These previously unknown terms are relevant for superconductors which contain heavy elements or have a small coherence lenght. The effect of the spin-orbit terms on dichroism in superconductors is investigated. It turns out that there are three ways to produce dichroism in a superconductor: (i) external magnetic fields (Faraday/Kerr effect), (ii) internal magnetic fields (magnetic superconductors) and (iii) unconventional order parameter. In all three cases the effect of the new off-diagonal terms is an additional contribution to the total dichroism below the critical temperature.

Orbital and Spin Magnetic Moments from Soft-X-ray Magnetic Circular Dichroism

C. T. Chen

AT&T Bell Laboratories, 600 Mountain Avenue, Murray Hill, NJ 07974, USA

High precision, $L_{2,3}$-edges photoabsorption and magnetic circular dichroism spectra of iron and cobalt were measured by the transmission method with in-situ grown thin films, eliminating experimental artifacts encountered by the indirect methods used in all previous measurements. The magnetic moments determined from the integrals of these spectra, according to the x-ray magnetic circular dichroism sum-rules, are found to be in excellent agreement (within 3%) for the orbital to spin moment ratios, and in good agreement (within 8%) for the individual moments, with those obtained from Einstein-de Haas gyromagnetic ratio measurements, demonstrating decisively the applicability of the individual orbital and spin sum-rules to these two itinerant magnetic systems. The general verification and applicability of the individual sum-rules to magnetic systems and the caveats for total electron and fluorescence yield x-ray magnetic circular dichroism measurements will be discussed.

Spin and orbital moments in rare earth ferromagnets

M. J. Cooper

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Magnetic Compton scattering is a technique that allows the spin-dependent momentum distribution in ferromagnets to be studied [1]. In alloys and compounds that contain dissimilar elements the momentum distribution of the electrons with unpaired spins are sufficiently different to allow the site specific spin moments to be separated from each other. This has been demonstrated in rare-earth compounds such as $HoFe_2$, $ErFe_2$ and $DyFe_2$ [2]. The spin moments can be followed as a function of temperature leading to the direct observation of spin compensation temperatures in compounds with antiferromagnetic coupling between the two sites [3]. In addition if the data on spin moments are combined with bulk magnetisation results some statement about the orbital component can be made.

The experiments reffered to above have been largely concerned with exploring the scope of this new technique and the actual moments in these materials are considered to be well-known. However measurements have recently been made on $CeFe_2$ where there is a pronounced difference between the calculated 4f moment [4] and that deduced from neutron data [5]. Our results show that the Ce 4f moment is very small - less than 0.1 μ_B which is in agreement with the neutron result and markedly different to the calculated value which is some four times larger. On the other hand the Ce 5d moment is higher than that inferred from the neutron measurement. These data together with those for UFe_2 will be discussed.

[1] Cooper et al. J Phys Condensed Matter **4** L399 1992

[2] Lawson et al. J Phys Condensed Matter **7** 389 1995

[3] Cooper et al. Phys Rev Letts. **71** 1095 1993

[4] Eriksson et al. Phys Rev Letts. **60** 2523 1988

[5] Kennedy et al. J Phys Condensed Matter **5** 5169 1993

Multiple scattering approach to magnetic dichroism in electron spectroscopy of transition metal systems

H. Ebert, J. Schwitalla and G. -Y. Guo

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A rigorous and parameterfree description of magnetic X-ray dichroism (MXD) and other related phenomena requires to deal with magnetism as well as relativistic effects on equal footing. A corresponding description of the electronic structure within the framework of spin-density functional theory is sketched in short. As a first step to go beyond this scheme inclusion of the magnetic interaction is discussed. To allow for a detailed discussion of the role of spin-orbit coupling a model Hamiltonian to be used within multiple scattering schemes has been derived that allows to scale the spin-orbit coupling strength without affecting other relativistic effects. Corresponding calculations of orbital magnetic moments MOKE- as well as MXD-spectra demonstrate the usefulness of the approach. Finally theoretical MXD-spectra in Cu-Co-alloys will be presented and discussed in some detail.

Spin polarisation of conduction electrons in metallic multilayers and intermetallic compounds evidenced by X-ray Magnetic Circular Dichroism

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After a delay of almost a century, synchrotron radiation has been able to associate the original ideas on magnetism of Zeeman and the discovery of X-rays by Röntgen. In the hard X-ray range, it is possible to produce polarisation-tunable sources using an additional optical device, the phase plate which opens up new classes of X-ray spectroscopies and new resonant methods of diffraction for magnetic materials. The main lines of X-ray magnetic circular dichroism at K-edge of the 3d elements, are discussed in term of hybridisation of the 4p-probed band with the spin polarized and orbital momentum-polarized d

band. Results on very appealing materials such Cu-Co, Cu-Fe multilayers which exhibit large magnetoresistance are presented in term of spin polarisation of conduction electrons of the copper layer. XMCD of Co/Cu and Fe/Cu multilayers at the copper K edge shows:
i) that the p-band of copper is significantly spin-polarised by the adjacent Co or Fe atoms;
ii) that the spin-polarisation of the copper layers strongly depends on the adjacent magnetic layer;
iii) that the magnetic polarisation is not restricted to the interface layer i. e. it departs from a simple $1/t_{\mathrm{Cu}}$ dependence.

Treating Electronic Excitations in Magnetic Materials by Solving Fully Relativistic Two-Component One-Particle Equations

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As has been shown in a number of articles by the present author, the Kohn-Sham version of density functional theory can be extended to stationary excited N-electron states which amounts to self-consistently solving N one-particle equations that have primarily the form of Dirac equations. Within rather lenient assumptions it is possible to reduce these equations to two-component equations without resorting to Foldy-Wouthuysen transformations. Hence, these equations hold to any order of v^2/c^2, different from the familiar relativistic Pauli equations. They contain an explicit expression for the spin-orbit coupling in the general case of magnetic order and offer the advantage - among other favorable aspects of numerical convenience - that they reduce in the limit $c \to \infty$ to a pair of one-particle Schrödinger equations for the two spin orientations. The capabilities of the new approach are demonstrated by results on collision induced spin polarization of low energy electrons that are scattered by heavy atoms.

Magnetic circular dichroism in x-ray fluorescence: experiment

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Universit Pierre et Marie Curie, 11 rue P. et M. Curie, 75231 Paris Cedex 05, France

Strange et al (Phys Rev Lett 1991) predicted that magnetic circular dichroism in x-ray fluorescence spectra (XFS) would measure the spin polarisation of valence states in a magnetically oriented ferromagnet. The appeal of such an experiment is that it may provide information concerning spin polarised hybridisation in magnetic alloys which, unless the component valence states are well separated, is not readily available even from spin polarised photoemission. A technical point of interest also is that XFS is relatively insensitive to surface effects which is of importance when dealing with composite magnetic

materials. We will present the data measured so far and discuss some of the outstanding problems related, either to the low efficiency of the experiment, or to the multielectron effects inherent in the excitation spectra. Some future experiments will be outlined.

Angular dependent magnetic dichroism in core level photoemission

U. Hillebrecht
Universität Düsseldorf

The use of linearly polarized light greatly facilitates studies of magnetic dichroism in core level spectroscopy. If one uses a chiral geometry in angle- resolved photoemission (MLDAD), the information obtained is identical to that contained in circular dichroism studies. The 3p and 2p levels of the 3d ferro- magnets have been studied in this way, supplemented by spin-resolved photoelectron detection. In such "complete" experiments the effects of exchange and spin-orbit interaction can be separated. Studies of the angular dependence of Fe and Co 3p MLDAD showed the influence of both the atomic angle dependence as well as strong photoelectron diffraction effects. The latter arise due to a dependence of the scattering of the photoelectron on the angular momentum (l) and magnetic (m) character of the final state. The present status and prospects of combining photoelectron diffraction with magnetic dichroism will be addressed.

Nonlinear Magneto-Optical Response of Thin Ferromagnetic Films

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Institute for Theoretical Physics, Freie Universität Berlin, Germany

Nonlinear magneto-optics is a sensitive fingerprint of the electronic, magnetic and atomic structure of surfaces, interfaces and thin films. We present a theoretical study of the nonlinear magneto-optical Kerr-effect in Fe, which demonstrates how various electronic material properties can be extracted from the nonlinear Kerr spectrum. We derive its dependence on exchange interaction and magnetization. We show that the Kerr rotation angle in second harmonic generation (SHG) is enhanced by one order of magnitude compared to the linear Kerr angle. Using the full-potential LMTO method we calculate the thickness dependence of the nonlinear Kerr spectra of thin Fe(001) films. We demonstrate how this dependence can be used for the characterization of ultrathin films. The polarization dependence of the SHG yield shows sensitively the symmetry of surfaces and interfaces.

Magnetic Circular Dichroism in Photoemission from Lanthanide Materials

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We report on our investigation of magnetic circular dichroism (MCD) in photoemission (PE) from magnetically ordered lanthanide materials, in particular from single-crystalline films of Gd, Tb, and Dy metal [1-3]. Particularly large MCD effects are expected for well-resolved $4f^{n-1}$ PE multiplet spectra, amounting up to 93% for the $^8S_{7/2}$ component of the Tb-$4f^7$ PE spectrum, with 67% observed [2]. An application of this new effect to a quantitative measurement of the degree of circular polarization in the soft x-ray region is discussed. Large MCD effects were also observed in the 4d core-level PE spectra of Gd and Tb metal, which are well accounted for by an atomic many-particle description [4]. Some applications of this new element-specific tool to the study of surface and interface magnetism are discussed: (i)Magnetic properties of the close-packed (0001) surfaces of Gd and Tb metall, and (ii) Magnetic behavior of the hetero-magnetic interface 1 ML Eu/Gd(0001)[5].

[1] K. Starke, E. Navas, L. Baumgarten, and G. Kaindl, Phys. Rev. B **48**, 1329(1993).

[2] K. Starke, L. Baumgarten, E. Arenholz, E. Navas, and G. Kaindl, Phys.Rev. B**50**, 1317(1994).

[3] E. Arenholz, E. Navas, K. Starke, L. Baumgarten, and G. Kaindl, Phys. Rev. B**51**, xxx (1. April 1995).

[4] G. van der Laan, E. Arenholz, E. Navas, A. Bauer, and G. Kaindl, Preprint (1995).

[5] E. Arenholz et al., to be published.

This work was supported by the BMFT, project 05-5KEAXI-3/TP01, and the DFG, Sonderforschungsbereich 290/TP A06.

X-ray Absorption in a Tight-binding Band Structure Approach

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We report the calculation of the X-ray Absorption Spectrum (XAS) and Circular Magnetic X-ray Dichroism (CMXD) at the L_3-edge of Dysprosium hcp metal. Using a LMTO-tight binding band structure method, we study dipolar (E1) core hole absorption to wide band final states. For heavy Rare Earth (RE) compounds, the LSDA prescription results in the

4f minority spin states being pinned at the Fermi level. Without spin-orbit coupling there is no orbital moment and the spin moment is incorrect. Spin-orbit coupling induces an orbital polarization of the 4f single particle eigenstates, with orbital and spin moments close to those of the corresponding RE ion in its Hund's rule ground state. Adding a Coulomb repulsion term to the unoccupied 4f diagonal elements of the Hamiltonian matrix, we shift these states to energies well above the Fermi level to obtain integer occupation of the 4f shell and correct spin moments for the 4f and 5d shells. To account for quadrupole (E2) absorption to the narrow 4f final states we use an atomic multiplet model for a Dy^{3+} ion. Combining E1 and E2 transitions, while accounting for their different dependence on the angle between the incoming photon wave vector and the magnetization direction, we explain the result of recent experiments, thus establishing the E2 nature of the negative feature at the low energy side of the Dy CMXD spectrum.

Spin-orbit transmission effects in the Kerr spectra of compounds: an ab initio study

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The magneto-optical (MO) Kerr spectra of a number of transition-metal and uranium compounds are studied from first principles, using density-functional band-structure theory. The theoretical Kerr spectra of the following transition-metal compounds will be discussed: (a) the Heusler alloys NiMnSb, PdMnSb, PtMnSb, PtMnSn, and Co_2HfSn, (b) the XPt_3 compounds, with X=V, Cr, Mn, Fe, and Co, (c) the layered MnPt, FePt, and CoPt compounds, (d) the hexagonal MnAs, MnSb, and MnBi compounds, and (e) some Invar alloys. Furthermore, the uranium monochalcogenides US, USe, and UTe are investigated, as well as some ternary uranium intermetallics. For the Heusler alloys, band-structure theory gives a very good description of the measured Kerr spectra. Particularly the giant Kerr rotation found experimentally in PtMnSb is straightforwardly obtained. The Kerr spectra of the layered XPt (X=Mn, Fe, Co) alloys are given for the (001), (111), and (110) orientation of the magnetic moment. Large Kerr anisotropies are predicted in these materials. For some of the XPt_3 compounds, theory also predicts a giant Kerr rotation. The origin of the large Kerr effect is analyzed by artificially changing the magnetic moments, the spin-orbit coupling strength, and the optical transition-matrix elements on each site. This reveals which interband transitions are responsible for the Kerr rotation peak, and that the large Kerr rotation is caused by a combination of the spin-orbit coupling on Pt and the magnetic moment on X. In case of the uranium compounds, the height and over-all shape of the Kerr spectra is satisfactorily given by the single particle LSDA approach. But when $5f$ electrons participate in the optical transitions, the detailed agreement becomes less good. Thus, while the LSDA does a perfect job for the MO spectra of transition-metal compounds, for the uranium compounds we come to the

limits of what can be described within the LSDA.

Relativistic Effects on Nuclear Quadrupole Coupling

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Relativistic effects strongly influence the NMR or hyperfine properties (chemical shifts, nuclear spin-spin coupling and nuclear quadrupole coupling) of atoms, molecules or solids. As first shown by Casimir in 1936 [1], for the two states $j = l \pm s$, three radial electric field gradient integrals, q_{++}, q_{+-}, and q_{--} must be introduced. The relativistic correction factors, defined for operator $\hat{q}$ as

$$C =< \mathrm{R}|\hat{q}|\mathrm{R} > / < \mathrm{NR}|\hat{q}|\mathrm{NR} >,$$

have quite different values for the three combinations. *E.g.* for the bismuth atom ground state 6p shell at Dirac-Fock level, C_{++} and C_{+-} are 1.28 and 1.91, respectively, while q_{--} vanishes entirely, due to $j = 1/2$. There also is a dependence on the n quantum number [2]. In addition to these relativistic changes of the integrals (at the atomic centre), *spin-orbit tilting effects* may occur, even at light atoms, bonded to heavy ones.

Electric field gradients have been observed in half-closed-shell atoms, whose $S > 1/2$, in free space and on cubic crystal sites. Examples are the p^3 , d^5 or f^7 atomic systems such as N – Bi, Mn and Mn^{2+} or Gd^{3+}. The value of q grows faster than Z^6, from 1.27 Hz to 305.067(2) MHz for the series from N to Bi. The nature of the effect was first understood by Sandars [3]. Similar effects are known in cubic, magnetic solids.

We have produced Dirac-Fock-level electric field integrals for the elements 1–94, investigated the hydrogen-like, n-dependent correction factors, C and used simple molecular-orbital models for estimating the spin-orbit tilting effects [4].

[1] H.B.G. Casimir *On the Interaction between Atomic Nuclei and Electrons*
Teyler's Tweede Genootschap, Harlem, 1936.
[2] P. Pyykkö, E. Pajanne and M. Inokuti, *Int.J. Quantum Chem.* **7** (1973) 785
[3] L. Evans, P.G.H. Sandars and G.K. Woodgate, *Proc. Roy. Soc. London* **A 289** (1965) 108.
[4] P. Pyykkö and M.C. Seth, unpublished results.

Linear magnetic dichroism in angle-resolved photoemission from Co(0001) ans Fe(110) valence bands

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The linear magnetic dichroism in the angular distribution of photoelectrons (LMDAD) from the valence bands of bulk-type epitaxial layers of Co(0001) and Fe(110) on W(110) has been studied by angle-resolved photoemission in the photon energy range from 14eV to 64eV.

For Co(0001) the LMDAD appears only near the crossing points of nonrelativistic Λ^3 and Λ^1 bands along the $A\Gamma$ direction of the first Brillouin zone.

A simple model is presented which interprets the LMDAD as follows: a) Near such a crossing point the states are $\Lambda^1\Lambda^3$ hybrids induced by the spin-orbit coupling. b) The photoelectron waves, emitted coherently from the Λ^1 and the Λ^3 part of the hybrid into a Λ^1 final state, interfere with a phase difference, which depends on the direction of the magnetization, thus causing the LMDAD.

The LMDAD of Fe(110) is interpreted in the framework of this model. The observed LMDAD can be explained by the formation of two $\Sigma^{1\downarrow}\Sigma^{3\downarrow}$ hybrids from bands with mainly $\Sigma^{1\downarrow}$ and $\Sigma^{3\downarrow}$ character and two corresponding $\Sigma^{1\uparrow}\Sigma^{3\uparrow}$ hybrids. We found that a) the LMDAD of the $\Sigma^{1\downarrow}\Sigma^{3\downarrow}$ hybrids possesses the opposite sign of the exchange-split $\Sigma^{1\uparrow}\Sigma^{3\uparrow}$ hybrids. b) The LMDAD-asymmetry of these hybrids shows a strong dependence on the photon energy with a maximum at about 26.7eV, such that the LMDAD varies for the same initial states but different final states. c) We found no hints for a hybridization between states of Σ^1 and Σ^3 symmetry but different spin character.

This work has been supported by the DFG / SFB 341 and the BMBF (FKZ: 05 5PCFXB 2).

Imaging of Magenetic Domains by means of Magnetic Dichroisms: Magnetic Spectro-Microscopy

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Multi-component thin film systems are of growing interest in magnetism with respect to both reasearch and application. They exhibit fascinating effects such as the oscillatory magnetic exchange coupling and the giant magnetoresistance. In order to arrive at a better understanding of these magnetic properties and the contributions from the individual components, an element-specific characterization is mandatory. This is particulary true for the magnetic microstructure. We have therefore developed a technique allowing an element-specific imaging of the magnetic domains of the different components in thin film systems. The technique is based on the magnetic circular dichroism (MCD) in the emission of photo- and secondary electrons, which is observed with excitation by circularly polarised synchrotron radiation. By tuning the energy of the radiation to the absorption edges of the respective material and by using Auger electrons for the imaging, one yields both elemental selectivity and surface sensitivity, which is an essential prerequisite for studying thin film systems. The various contrast mechanisms due to different magneto-dichroic effects will be discussed, and first applications to the Fe/Cr system will be shown.

The work was supported by the Bundesministerium f. Forschung u. Technologie (grants No. 055EFAAI5 and No. 055VHFX1)

On the Interpretation of MXCD Experiments on Itinerant Magnets

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The famous sum rules derived by Thole, Carra, Altarelli and coworkers have provided a unique insight into localized magnetism and have enabled us to use absorption dichroism measurements to make an approximate determination of the orbital and spin contribution to the magnetic moment of a material separately. In this talk I will present a new rule for comparing absorption dichroism experiments directly with band theory. We are able to show a direct proportionality between the dichroism and the total magnetic moment of the $j = l - 1/2$ electron states above the fermi energy. i.e. Dichroism experiments enable us to determine the total magnetic moment of the $j = l - 1/2$ conduction electron states separately from the total moment of the $j = l + 1/2$ states. The new rule does not require an energy integration and all the required parameters can be calculated easily from relativistic spin-polarised band theory. This theory will be illustrated with applications at the L_2 edge in pure Fe and in the random substitutional alloy $\mathrm{Fe}_{80}\mathrm{Co}_{20}$.

Magnetic Ground State Properties and Angular Dependent Magnetic Dichroism in Core Level Photoemission

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Angle dependent core level photoemission excited with polarized x-rays can be used to determine the magnetic properties of metallic systems by separating the geometrical dependence from the physical information which is contained in the spectra. There are four different geometries which can be distinguished: magnetic circular dichroism (MCD), linear dichroism (LD), circular dichroism in the angular dependence (CDAD), and magnetic linear dichroism in the angular dependence (MLDAD). The shape of the dichroic spectra in a one-electron model is determined by the core spin-orbit interaction and the spin field. A good agreement between experiment and theory is obtained for the Fe 3p photoemission of iron when the spin and orbit dependence of the life time broadening is taken into account. The influence of the orbit field and the spin filtering in the solid can be estimated

from the first spectral moment.

Relativistic AES

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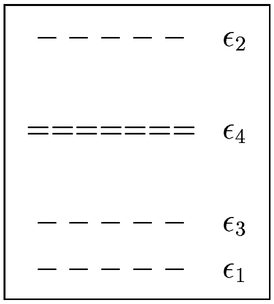
Inst. für Techn. Elektrochemie, TU Wien, Getreidemarkt 9, A-1060 Wien

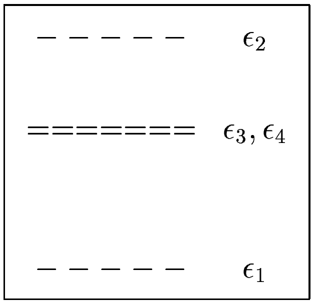
Non-spin-polarized and spin-polarized relativistic core-core-valence (ccv)-

$\psi_1(\mathbf{r}_1)$	core state#1	:	ϵ_1
$\psi_2(\mathbf{r}_2)$	continuum state	:	ϵ_2
$\psi_3(\mathbf{r}_3)$	core state#2	:	ϵ_3
$\psi_4(\mathbf{r}_4)$	valence state	:	ϵ_4



and core-valence-valence (cvv) relativistic AES theory

$\psi_1(\mathbf{r}_1)$	core state	:	ϵ_1
$\psi_2(\mathbf{r}_2)$	continuum state	:	ϵ_2
$\psi_3(\mathbf{r}_3)$	valence state	:	ϵ_3
$\psi_4(\mathbf{r}_4)$	valence state	:	ϵ_4



as based on local spin density functional approximations is discussed for semi-infinite solid systems, i. e. , for systems with surfaces. It will be shown that the selection rules are in general governed by the following scheme:

	Degeneracy			$\mathbf{D}^2$	$\mathbf{E}^2$	**DE**
	Core WF $\psi_1(\mathbf{r}, \epsilon_1)$	Core WF $\psi_3(\mathbf{r}, \epsilon_3)$	Cont WF $\psi_2(\mathbf{r}, \epsilon_2)$			
no magnetic field	μ_1	μ_3	μ_2	$3j$	$3j$	$6j$
with magnetic field	–	–	–	$9j$	$9j$	$12j$

and that the intensity can be expressed as

$$\overline{P} = \sum_n \exp(-\gamma d_n) \overline{P}^n \quad ,$$

where the $\overline{P}^n$ are layer-dependent transition probabilities, d_n the separation between the layers and γ is proportional to an escape length.

Magneto Optical Kerr Effect in Strongly Anisotropic Magnetic Thin Films: FePt and Co

D. Weller

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Magneto-optical (MO) effects both in the visible and in the x-ray regime are powerful experimental methods to study magnetic and electronic properties of thin film materials as are being used in magnetic and magneto-optic recording. Of the various important materials parameters we have specifically investigated the electronic underpinnings of the magneto-optical Kerr effect (MOKE), which is used in MO recording to read back the stored bit information. In model systems like epitaxial Co and FePt superlattice films grown in different crystallographic orientations, we demonstrate that there exists a strong correlation between the magnitude of MOKE and the occurrence of magneto-crystalline anisotropy (MCA). Up to 100% changes in Kerr rotation and ellipticity are observed, as the orientation is changed from (001) to (110) in FePt (CuAu(I)) compound films. While the (001) film has a strong out-of-plane anisotropy with anisotropy fields of the order of ~80 kOe, the (110) film has an in-plane easy axis with anisotropy of similar strength and large coercivity of $H_C \sim 7$ kOe, which makes this an interesting material for magnetic recording applications. The observed Kerr effect enhancement occurs in the (001) direction, that means for the case of a parallel alignment of photon propagation and MCA axis.

work done with G.R. Harp, A. Cebollada, A. Carl and R.F.C. Farrow; see D. Weller et al., Phys. Rev. Lett. 72, 2097 (1994).

Report on collaborative visit of H. Ebert (München) to W. M. Temmerman, Z. Szotek and G.-Y. Guo (Daresbury), 26th - 30th March, 1995

During the last years there was a very fruitful collaboration of the Daresbury group with me. Our main tool was and still is the self-consistent spin-polarized relativistic LMTO (SPR-LMTO) package that has been developed together. Up to now the code is based on the ASA. Some years ago I developed a full-potential scheme, that is to some extent a mixture of the full-potential approch developed in Jülich by P.-H. Dederichs and R. Zeller as well as the full-potential version of the LMTO developed by S. Yu. and D. Yu. Savrasov. Implementation of that scheme in parallel and coordinated with the recent activities and interests of the Daresbury group have been discussed.

A further topic was the preparation of the new HCM-network "ψ_k-magnetism" and the first meeting of the interested collegues (20th April 1995 in Herrsching, Germany).

About half of my stay in Daresbury was devoted to discussions with G.-Y. Guo on recent results obtained with the SPR-LMTO package. G.-Y. Guo recently included the Dirac equation solver developed in Munich that allows to manipulate the spin-orbit-interaction into the program. First results have been obtained for the spin and orbital magnetic moments as well as the Kerr rotation spectrum of pure Ni. Furthermore an extensive study of the hyperfine fields in multilayers has been performed looking primarily to the anisotropy of the fields due to the orbital and dipolar contributions.

(H. Ebert)

HCM WORKSHOP WIEN95

Full-Potential LAPW Calculations with the WIEN95 Code

Technical University Vienna, Austria, April 19-22, 1995
Chairman: **K.Schwarz** (TU Wien)
SPONSORS:
Human Capital and Mobility Programme
Austrian Science Foundation (FWF)

The new version of the full-potential Linearized Augmented Plane Wave (FP-LAPW) method as embodied in the WIEN95 code has been developed mostly in Vienna but additional features, such as the calculation of forces, were implemented as a result of a fruitful collaboration with several groups, in particular those at the Fritz-Haber Institute (Berlin), Max-Planck-Institut für Metallforschung (Stuttgart), and the University of Graz. This HCM workshop lasted for four days and was attended by 54 researchers from 15 countries. The scientific programme covered a short introduction to Density Functional Theory, band structure methods in general and the LAPW method, with corresponding algorithms, in particular. The outline and handling of the new user-friendly program was described in detail by P.Blaha but the participants had also a chance to run WIEN95 on several workstations in five exercise sessions. One day was devoted to the calculation of forces. In addition to the part directly related to the WIEN95 package, lectures and posters illustrated many interesting band structure results such as generalized gradient corrections, electric field gradients, optical properties, crystal field parameters, energy loss spectra, elastic constants, magnetic properties, applications in mineralogy or materials science. We have received very positive reactions from the participants who told us that they had learned a lot and praised the balance of this workshop in terms of introduction, program handling, exercises and results. It was extremely useful and the participants clearly wanted to have a similar meeting in about a year. It can be expected that several interesting European collaborations will evolve from this workshop and new ones will be initiated.

The full list of participants is included below.

(K. Schwarz)

Dipl.Ing. Robert Abt (Univ. Graz, Austria)
Phys.Dipl. Paola Alippi (FHI, Berlin, Germany)

Dr. Claudia Ambrosch-Draxl (Univ. Graz, Austria)
Dr.Piotr Badziag (University College of Maelardalen, Sweden)
Jean-Luc Barras (Univ. Fribourg, Switzerland)
Dr. Lubomir Benco (IIC, Slovak Academy of Scienes, Bratislawa, Slovakia)
Doz.Dr. Peter Blaha (TU, Wien, Austria)
Dr.Gianluigi Botton (Univ. Cambridge, UK)
Prof.Dr.Tilman Butz (Univ. Leipzig, Germany)
Dr. Erich Deiss (ETH Zürich, Switzerland)
Anna Delin (Univ. Uppsala, Sweden)
Dr. Philipp Dufek (TU Wien, Austria)
Prof.Dr.Manfred Fähnle (MPIM Stuttgart, Germany)
Lars Fast (Univ. Uppsala, Sweden)
Mag. Elisabeth Gustenau (Univ. Wien, Austria)
Dr.Jenny Henderson (Univ. Trondheim NTH, Norway)
Dipl.Phys.Heike Herper (Univ. GH Duisburg, Germany)
Dipl.Phys.Egbert Hoffmann (Univ. GH Duisburg, Germany)
Dr. Randi Holmestad (Univ. Trondheim NTH, Norway)
Dipl.Phys. Carsten Holtfort (Univ. GH Duisburg, Germany)
Dipl.Phys. Harald Hutter (Univ. Dortmund, Germany)
Peter James (Univ. Uppsala, Sweden)
Phys.Dipl. Bernd Kohler (FHI, Berlin, Germany)
Robert Kouba (Univ. Graz, Austria)
Horst Krimmel (MPIM Stuttgart, Germany)
Dr.Estelle Kunoff (Ben-Gurion University, Israel)
Jessika Leydendecker (Humbolt Univ. Berlin, Germany)
Dr. Frantisek Maca (Czech Academy of Sciences, Prague, Czech Republic)
Dr.Samir Matar (ICMC Bordeaux-CNRS, France)
Dr.Peter Mohn (TU Wien, Austria)
Dr. Pavel Novak (Czech Academy of Sciences, Prague, Czech Republic)
Guilherme Nunes (INESC, Lisbon, Portugal)
Clas Persson (Linkoping University, Sweden)
Dipl.Phys. Carsten Pohlmann (Univ. Karlsruhe, Germany)
Dr.Ute Pustogowa (Freie Univ. Berlin, Germany)
Dipl.Phys.Alexander Quandt (Univ. Tübingen, Germany)
Dipl.Phys. Sven Quassowski (FHI Berlin, Germany)
Angel Rodriguez-Marco (Universidad Autonoma de Madrid, Spain)
Babak Sadigh (KTH Stockholm, Sweden)
Martin Schatzmayr (Linkoping University, Sweden)
Joachim Scheipers (TU München, Germany)
Mark Sifkovits (Univ. Dortmund, Germany)
Dr. Walter Schirmacher (TU München, Germany)

Dr. Andreas Schirmer (KFA Jülich, Germany)
Prof.Dr. Karlheinz Schwarz (TU Wien, Austria)
Dr.Valeri Smelyansky (SIMS, National Research Council of Canada, Ottawa)
Dipl.Phys. Holger Smolinski (Univ. Dortmund, Germany)
Dr. Mojmir Sob (IPM, Acad. Sci. Czech Republic, Brno)
Torsten Soldner (Univ. Leipzig, Germany)
Prof.Dr.Heinrich Sormann (TU Graz, Austria)
Dr.Andzej Szajek (IMP, Polish Academy of Sciences, Poznan)
Dr.Wolfgang Trger (Univ. Leipzig, Germany)
Dr.Björn Winkler (Inst. u. Museum, Univ. Kiel, Germany)
Jian-Min Zuo (Arizona State University, Tempe, USA)

Announcement

Postdoctoral Position

Geophysical Laboratory, Carnegie Institution of Washington,
5251 Broad Branch Road, N.W., Washington, D.C. 20015, USA

A postdoctoral position is available beginning in October or November 1995 in the field of first-principles studies of ferroelectrics. Experience in band structure methods and/or molecular dynamics is required. Please email vita and bibliography to **cohen@quartz.ciw.edu**.

(Ronald Cohen)

Announcement

Ph. D. Position

Ludwig-Maximilians-Universität München, Germany

There is one Ph. D. position available within the project on **"Zirkular polarisierte Synchrotronstrahlung: Dichroismus, Magnetismus und Spinorientierung"** of the German Ministry for Research and Technology (BMFT). The project is concerned with the *Relativistic Effects in the Spectroscopy of Magnetic Solids: AES, VB-XPS, core-level XPS, XAS, etc.*

All work will be based on the spin-polarized relativistic version of the KKR-method (multiple scattering theory), combined (where necessary) with the CPA.

Starting date: anytime

Salary: around 1600 DM (after tax) (BAT IIA/2) depending on age and number of wives and/or children

Contact:

Hubert Ebert, Prof. Dr.,
Inst. für Physikalische Chemie der
Ludwig-Maximilians-Universität München
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Ab initio study of tritium defects in lithium oxide

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† Now at IRRMA, IN-Ecublens, CH-1015,Lausanne, Switzerland

Abstract

Lithium oxide has been suggested as a suitable breeder blanket material for fusion reactors. Tritium ions and lithium vacancies are created by neutron irradiation, forming bulk defect complexes whose exact character is experimentally unclear.

We have used *ab initio* total energy pseudopotential methods to study the structure and relative energies of tritium as a substitutional defect, and of the separate tritium interstitial and lithium vacancy. For all stable defect geometries the formation of an OT^- complex with an O—T bond length of about 1Å is found to be energetically favoured. In the case of the substitutional defect this bond is found to point towards the vacant Li site, but the direction is fairly free for the interstitial case. The binding energy of tritium to a lithium vacancy is found to be 1.3eV. Structural relaxation effects are included throughout, and are found to significantly affect the relative energies of different defect geometries. The effects of zero-point fluctuations are estimated and found not to be very significant.

The most probable migration path of interstitial tritium is identified as a jump between nearest neighbour oxygen ions, with an activation energy of 0.45eV, in agreement with experimental evidence. The results suggest a picture of thermally assisted diffusion of tritium interstitials and lithium vacancies along the anion and cation sub-lattices respectively, with the preferential trapping of the two defects into substitutional complexes.

(submitted 27th April 1995 to J. Phys.: Condensed Matter)
Preprint available on request from Rajiv Shah (rs133@phy.cam.ac.uk)

Relativistic calculations of the magneto-optical Kerr spectra in (001) and (111) US, USe, and UTe

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Abstract

The magneto-optical (MO) Kerr spectra of the isochemical uranium compounds US, USe, and UTe are investigated from first principles, using density-functional theory in the local spin-density approximation and the relativistic ASW band-structure method. Fully relativistic, optical transition-matrix elements are derived from Dirac theory. The *ab initio* calculated Kerr spectra compare reasonably well with experimental spectra in height, but the theoretical spectra exhibit a double peak structure, whereas the experimental ones show only one peak and a vague shoulder. To explain this difference, attention is first given to anisotropy effects related to the strong magnetic anisotropy present in these compounds. Polar Kerr spectra are calculated for two magnetization directions, the (001) and (111) (i.e. easy axis) direction. A clear anisotropy is found in the Kerr spectra of these two magnetizations, but the differences between experimental and theoretical spectra can not be related to the magnetic anisotropy. Secondly, the influences of the lattice spacing and of an external magnetic field on the Kerr spectra are investigated, but no explanation of the differences found can be derived thereof. The band structures and Kerr spectra obtained by the ASW method are furthermore checked by recalculating them with a fully relativistic LMTO scheme and are found to be essentially the same. The positions of the *ab initio* energy bands are in addition in accordance with experimentally determined band positions. The origin of the difference in the Kerr spectra is discussed in relationship to electron-correlation effects and to the orbital polarization.

(to appear in Phys. Rev. B)
Manuscript available on request from: peter@tmps08.mpg.tu-dresden.de

Theoretical study of the magneto-optical Kerr spectra of (001) and (110) XPt (X = Mn, Fe, Co)

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Abstract

The polar magneto-optical (MO) Kerr spectra of the layered bimetals MnPt, FePt, and CoPt are calculated for the (001) and (110) magnetization directions. A sizeable orientation dependence of the Kerr spectra on the magnetization axis is found. This Kerr anisotropy appears to coincide with the strong magneto-crystalline anisotropy found experimentally in FePt and CoPt multilayers, where the orientation of the magnetic moment perpendicular to the layers is favored. The origin of the magnitude of the Kerr effect and of the Kerr anisotropy is considered in relationship to the (001) and (110) orbital moments, the magnetocrystalline anisotropy energy (MAE), and the spin-orbit interaction. No clear relationship between the anisotropy in the orbital moments and that in the Kerr spectra is found. It is concluded that the optical transition matrices are mainly responsible for the Kerr anisotropy.

(submitted to Phys. Rev. B)
Manuscripts available from: peter@tmps08.mpg.tu-dresden.de

Surface core-level shifts of metal monolayers on transition metal substrates and their relation to the surface chemical reactivity

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Unter der Linden 6, D-10 099 Berlin
M.V. Ganduglia-Pirovano[1] and M. Scheffler
Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4-6, D-14 195 Berlin-Dahlem

Abstract

Using density-functional-theory we study the electronic and structural properties of a monolayer of Cu on the fcc(100) and (111) surfaces of the late 4*d* transition metals, as well as a monolayer of Pd on Mo bcc(110). We calculate the ground state of these systems, as well as the ionization energies of core electrons. The theoretical results are compared to available experimental data and discussed in a simple physical picture; it is shown how surface core-level shifts are related to the chemical reactivity of the adlayer.

Submitted Phys. Rev. Lett. May 1995
Latex-file can be obtained from: dxh@tanne.physik.hu-berlin.de or
vero@audrey.mpi-stuttgart.mpg.de

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Small Band Gap Semiconducting Polymers made from dye molecules: Poly-squaraines

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Philips Research Laboratories,
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Abstract

Small band gaps facilitate the use of polymers as semiconductors. Dye molecules can be used to construct semiconducting polymers with small band gaps. We use *ab initio* calculations to systematically design and study polymers based upon squaraine dyes. The calculated band gaps range from 2.7 eV to as low as 0.2 eV. Simple arguments based upon a Hückel analysis of the *ab initio* results enable us to identify the factors that control the size of the band gap. Squaraine polymers synthesized up till now fall into a class in which the band gap (≥ 1.3 eV) essentially reflects the HOMO/LUMO energy difference of the squaraine momomer fragment. We predict that a second class of polymer topology leads to much smaller band gaps. The reason for this is that band formation in the polymer shifts the energy of the highest occupied state of the polymer up with respect to the HOMO of the squaraine momomer, whereas the energy of the lowest unoccupied state of the polymer is fixed at the level of the monomer LUMO because of symmetry. New semiconducting polymers can be designed using such general principles as symmetry and topology.

(submitted *J. Am. Chem. Soc.*)
Preprint available on request from: brocks@prl.philips.nl

RELATIVISTIC FULL POTENTIAL PHOTOEMISSION THEORY FOR FERROMAGNETIC MATERIALS

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Abstract

The presented photoemission theory for ferromagnetic materials is a straightforward generalisation of the recently developed relativistic photoemission theory for space-filling cell potentials. On the basis of the one-step model we present a general scheme for photoemission calculations from ordered ferromagnetic systems. Therefore, the spin-polarized Dirac equation with a space-filling cell potential is solved, using the relativistic phase functional approach. The calculational scheme for the dipole operator and the spin-density matrix of the photocurrent is presented. This ansatz allows us to take spin-orbit together with exchange interaction into account, which for example is a basic requirement in calculating magnetic dichroic effects.

(submitted to Phys. Rev. B)
REVTEX version can be obtained from: mflucht@dosuni1.rz.uni-osnabrueck.de

Uniaxial and planar magnetic anisotropy of thin transition-metal films

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Abstract

We present in novel approach to the calculation of magnetic anisotropies in crystals and in thin films. Our technique is based on selfconsistent real-space recursion calculations on a tight-binding–linear-muffin-tin-orbital (TB-LMTO) - Hubbard Hamiltonian including spin-orbit coupling and allowing for arbitrary orientations of the local spin-quantization axes. It allows to scan the magnetic energy continuously as a function of the orientation of the magnetic moment and thus to avoid the computational problems that plague other techniques. Applications are presented for bulk body-centred cubic iron and for face-centred cubic Fe monolayers on Cu(100) and Cu(111) substrates. We predict a perpendicular direction of the magnetic moment for Fe/Cu(100) and in-plane orientation of the spins for Fe/Cu(111), with anisotropiy energies of the order of 1 to 2 meV/atom. The technique is accurate enough for studying the weak in-plane anisotropies in Fe/Cu(111) that are of the order of 1 μeV/atom.

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Preprints available from: jhafner@tph.tuwien.ac.at

Site-selective adsorption of C-atoms on Al(111) surfaces

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Abstract

Although carbon is a common contaminant of Al surfaces, neither its favourable adsorption sites, nor its bonding and electronic properties are known or understood to date. In this paper we report on density-functional theory calculations for this system which identify two nearly degenerate adsorption sites: *i* an "fcc-type" sixfold coordinated site half way betwen the first and second Al layer and *ii)*a "hcp-type" fourfold-coordinated site slightly below the surface layer. We argue that only the C adatoms at the "hcp-type" sites have been detected in recent scanning tunneling microscopy experiments, but predict that the "fcc-type" C-adatoms should exist in thermal equilibrium as well.

Physical Review Letters (in print)
Preprints available from: jhafner@tph.tuwien.ac.at

Dimer reconstruction and electronic surface states on clean and hydrogenated diamond (100) surfaces

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Abstract

We present ab-initio investigations of the structural and electronic properties of clean and hydrogen-covered diamond (100) surfaces within local-density-functional (LDF) theory. Our calculations are based on a variational solution of the Kohn-Sham equations using a preconditioned conjugate-gradient approach and on the optimization of the atomic structure via a quasi-Newton quench based on the exact Hellmann-Feynman forces. The computations are performed in a plane-wave basis, the electron-ion interaction is described by optimized ultrasoft pseudopotentials. We find that the clean and the monolayer-covered surfaces reconstruct in a (2×1) cell via the formation of rows of symmetric π-bonded dimers. Further hydrogenation to a coverage of 1.5 monolayers stabilizes a surface with a (1×1) periodicity in the C-layers, albeit with a low H-desorption energy for the formation of the reconstructed monohydride surface. The two-step desorption process is in good agreement with experimental observations. Electronic surface states within the bulk gap are predicted for the clean surface, but not for the monohydride case. The detailed analysis of the layer-resolved local densities of states and of the dispersion of the surface states demonstrates that the results are in good agreement with recent photoemission experiments. A negative electron affinity is predicted for the monohydride-surface, but not for the clean surface.

Physical Review B (submitted)
Preprints available from: jhafner@tph.tuwien.ac.at

ELECTRONIC STRUCTURE OF ICOSAHEDRAL AND DECAGONAL AL-PD-MN ALLOYS

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Abstract

We present calculations of the electronic structure of icosahedral and decagonal Al-Pd-Mn alloys, based on a hierarchy of rational approximants to realistic quasicrystalline structures and the linear-muffin-tin-orbital (LMTO) and tight-binding LMTO methods. For the icosahedral phase we show that a structure-induced density-of-states minimum at the Fermi-level exists for the stable 2/1 and all other higher-order approximants, but not for the lowest-order 1/1 phase. We also present preliminary results for the decagonal phase and show that the electronic structure is similar to that of the icosahedral alloy.

(Submitted to 5th Intern. Conference on the Physics of Quasicrystals (Avignon, May 1995))
Preprints available from: jhafner@tph.tuwien.ac.at

Electronic structure of crystalline and amorphous Nb_xMo_{1-x} alloys: Rigid versus rectangular bands

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Abstract

Ab-initio investigations of the electronic structure of disordered body-centred cubic and of amorphous Nb-Mo alloys are presented. We find that the crystalline Nb-Mo alloys are a rare example of an alloy system that conforms with the expectations of the rigid-band model. The electronic density of states of the amorphous Nb-Mo alloys differs drastically from that of the crystalline phases: it is rather close to the simple Friedel-model of a rectangular density of states. The origin of the striking differences in the band-structure and their consequences for the electronic properties, e.g. Collver-Hammond correlation in the superconducting transition temperatures, are discussed.

Submitted to J.Phys.:Condens.Matter
Preprints available from: jhafner@tph.tuwien.ac.at

The structural and electronic properties of rhodium surfaces: An ab-initio approach

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Abstract

The structural and electronic properties of the low-index surfaces of Rhodium have been investigated via fully self-consistent *ab-initio* local-density-functional (LDF) calculations. Our technique is based on ultrasoft pseudopotentials, a preconditioned conjugate-gradient technique for the calculation of the electronic ground-state and of the Hellmann-Feynman forces and stresses, and on a conjugate-gradient technique for the optimization of the atomic structure. The calculations were performed for five- to ten-layer slabs in symmetric and asymmetric geometries, allowing for the relaxation of up to seven surface layers. For the (111), (100), and (111) surfaces an inward relaxation of the top layer by -1.7 ± 0.2, -3.8 ± 0.2, and $-9.8 \pm 0.6\%$ is predicted, the surface-energies increase parallel to the inward-relaxation. The analysis of the electronic structure shows that the inward-relaxation is caused by the de-population at the surface of anti-bonding states at the top of the d-band. We also present a detailed analysis of electronic surface states.

Submitted to Surface Science.
Preprints available from: jhafner@tph.tuwien.ac.at

Theory and convergence properties of the screened Korringa-Kohn-Rostoker method

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Abstract

Within the framework of the generalized multiple-scattering theory, a conceptually clear and transparent derivation of the real-space screened Korringa-Kohn-Rostoker method is presented. It is suggested, that by a suitable choice of the reference system, a fast exponential spatial decay of the structure constants can be obtained. This opens the way to treat large-scale systems in real-space with a computational complexity that scales more favorably than the usual increase with the third power of the number of atoms.

(submitted to Phys. Rev. B)
The revtex-file and postscript figures are available from: Ru.Zeller@kfa-juelich.de

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Electronic structure and phase stability of three series of B2 Ti-transition metal compounds

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Abstract

Self-consistent electronic structure calculations have been performed for the twelve B2-TiM compounds (M=Fe,Co,Ni,CU; Ru,Rh,Pd,Ag; Os,Ir,Pt,Au) using the linear muffin-tin orbital (LMTO) method. The calculated lattice constants and bulk moduli are in good agreement with measurements. An analysis of the possible correlations between the instability of the B2-structure and the electronic structures of the 12 TiM compounds has been carried out. The sequence of the B2 phase instabilities and the cubic-¿orthorhombic (or monoclinic)-¿orthorhombic (or monoclinic)-¿tetragonal tendency in the three TiM series have been discussed in terms of band filling effect. The possible driving mechanisms of the structural phase transitions in the TiM series have been analysed based on the results of the generalized susceptibility $X_0(q)$ calculations.

J. Phys.: Condensed Matt., (in press) (1995)
Preprints available from g.y.guo@dl.ac.uk

Plasmon dispersion and broadening in A_3C_{60} (A=K, Rb)

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Abstract

Inelastic electron energy loss measurements of the 0.5 eV charge carrier plasmon in K_3C_{60} are presented, showing that the plasmon has a very large broadening but a negligible dispersion. The response function is calculated in a self-consistent, conserving approximation, showing that the plasmon broadening can be explained in terms of a decay in an electron hole pair under the emission of phonon(s). The plasmon dispersion can be understood within the random phase approximation. Local-field effects tend to give a large negative dispersion, which is compensated by interband effects.

(submitted to PRL)
Preprints available from: gunnar@radix3.mpi-stuttgart.mpg.de

Plasmon dispersion in A_3C_{60} (A=K, Rb)

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Abstract

We present experimental and theoretical results for the dispersion of the 0.5 eV charge carrier plasmon in A_3C_{60} (A=K, Rb) compounds. The experimental dispersion in K_3C_{60} is zero within the experimental accuracy, and the theoretical dispersion is slightly negative. We show that the small dispersion results from two large, opposing effects. Local-field effects tend to lead to a large negative dispersion, while interband transitions largely cancel this effect. The interband effects can be thought of in terms of the dielectric function due to classical, polarizable spheres describing the C_{60} molecules. This dielectric function reduces the plasmon energy, and the reduction of the dielectric function with increasing q tends to lead to a large, positive dispersion.

(submitted to PRB)
Preprints available from: gunnar@radix3.mpi-stuttgart.mpg.de

Plasmon damping and dispersion in doped C_{60} compounds

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Abstract

Inelastic energy loss measurements of the 0.5 eV charge carrier plasmon in K_3C_{60} are presented, showing that the plasmon has a very large broadening but a negligible dispersion. The response function is calculated in a self-consistent, conserving approximation, showing that the plasmon broadening can be explained in terms of a decay in electron hole pair(s) under the emission of phonon(s). The negligible plasmon dispersion can be understood within the random phase approximation. Local-field effects tend to give a large negative dispersion, which is compensated by interband effects.

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Optical Properties studied using Linear Muffin Tin Orbital Theory

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Abstract

A new method is presented for calculating optical properties within the framework of the self consistent Linear Muffin Tin Orbital (LMTO) band structure theory. We show how Green's second identity along with the commutation relation between the position and Hamiltonian operators may be used to calculate gauge independently the velocity matrix elements required for optical properties. The method has been applied to calculate the imaginary part of the dielectric function $\epsilon_2(E)$ for FeSi and Si. Notably, the new expressions for matrix elements are also valid for Hamiltonians in which nonlocal potentials are included.

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Preprints available from: dhobbs@alice.phy.tcd.ie

Possibility of various magnetic configurations in the Cr (Fe) monolayer deposited on vicinal surfaces of Fe (Cr)

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Abstract

The local magnetic moments and magnetic order are calculated for a Fe (Cr) monolayer adsorbed on semi-infinite Cr (Fe) substrates with high index surfaces. These stepped interfaces are present in the "wedge-shaped" configurations recently analyzed by different experimental groups in order to investigate the interlayer magnetic coupling in Fe/Cr/Fe systems. The spin-polarized electronic distribution is obtained by solving self-consistently a d-band model Hamiltonian in the mean field approximation within the framework of the tight-binding real-space method. Several magnetic configurations have been found for all the systems investigated. In the most stable configuration of the Cr monolayer on Fe vicinal surfaces, the local moments of most of the Cr atoms are antiferromagnetically coupled with the Fe moments, an exception being the Cr atoms at the edge of the step. Cr atoms at nearest neighbor positions (located at the kink and edge of the steps) are always antiferromagnetically coupled. For the Fe monolayer on Cr vicinal surfaces, the average magnetization at the surface results in zero for the two most stable solutions. However, other metastable solutions with net average magnetization on the Fe overlayer are found. The Fe atoms at the edge and kink of the steps (first neighbors) are, in all cases, ferromagnetically coupled. These results are in qualitative agreement with recent experimental observations.

(Phys. Rev. B (in press))
Complete paper available from: vega@fixat8.fam.cie.uva.es

Magnetic order transition in thin Fe overlayers on Cr: role of the interfacial roughness

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Abstract

The distribution of magnetic domains in a thin Fe overlayer on Cr is calculated as a function of the coverage-thickness in the presence of roughness at the interface. The spin-polarized electronic structure is determined by solving self-consistently a d-band model Hamiltonian in the mean field approximation. Arising from a magnetic multi-domain arrangement, a zero total magnetic moment is obtained when starting the Fe deposition. A transition towards a single Fe domain at a critical coverage-thickness leads to a net magnetization in qualitative agreement with various experimental observations. This macroscopic magnetic behavior is traced back to environment-dependent microscopic properties such as the local magnetic moments and magnetic ordering.

(submitted to Europhysics Letters)
Complete paper available from: vega@fixat8.fam.cie.uva.es

Spin polarization of Mn layers on Fe(001)

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Abstract

The spin polarization of Mn layers for a body-centered-tetragonal structure on Fe(001) is studied using a self consistent tight-binding real space model within the unrestricted Hartree-Fock approximation to the Hubbard Hamiltonian. We investigate all the possible magnetic structures of Mn overlayers with respect to the Fe majority-spin direction as a function of the exchange integral J of Mn. For an antiparallel alignment of a Mn monolayer with the ferromagnetic Fe substrate, the Mn magnetic moment exhibits a second order transition from low-spin to high-spin in large interval of the exchange integral J ($0.35 \leq$J$\leq 0.85eV$). The parallel Fe-Mn arrangement exists only for the high-spin ($J > 0.49eV$), whereas for $J \leq 0.49eV$ this solution undergoes a first order transition towards the antiparallel Fe-Mn. Interesting cases are obtained for thicker Mn slabs, which show different solutions for all possible interlayer magnetic arrangements of Mn as function of the interfacial Fe-Mn spin alignment. The Mn shows a tendency to form layer-by-layer antiferromagnetic structure coupled ferromagnetically with the ferromagnetic Fe substrate.

(submitted to Phys. Rev. B)
Complete paper available from: said@fixat8.fam.cie.uva.es

On the origin of orbital magnetization and magnetocrystalline anisotropy in TX ordered alloys (where T = Fe, Co and X = Pd, Pt)

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Abstract

We present a method to calculate the magnetic anisotropy parameters which is based on a perturbative treatment of the spin-orbit interaction and a Green's functions technique in real space. It allows to interpret the magnetocrystalline anisotropy energy (MAE) in terms of interatomic interactions in the crystal. The method is applied to analyse orbital magnetism and MAE in TX ordered alloys (where T=Fe, Co and X=Pd, Pt). The convergency of the orbital moments and MAE in real space and its relation to the problems of Brillouin zone integration and of oscillatory behavior of MAE as a function of band filling are discussed. A comparison with results obtained by other methods is also given.

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Dipole waves in tetrahedral semiconductors: bulk silicon

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Abstract

The connection between bond polarisability, local fields and the dielectric function of bulk silicon is investigated using bond polarisabilities and bond interaction tensors from ab initio cluster calculations. The static dielectric function is obtained as a function of bond polarisability using point dipolar local fields and local fields corrected at short range for the finite size of a bond. Comparison is made to the Clausius-Mossotti relationship between dielectric function and polarisability. The frequency-dependent dielectric response in the long wavelength limit is formulated in terms of longitudinal and transverse dipole waves. These are obtained by treating the electrons as a lattice of oscillators with coupling via the local fields. The dispersion relation for the dipole waves is calculated and waves corresponding to optical transitions and bulk plasma oscillations are identified. Dipole wave methods for calculating dielectric response properties of solids, including optical properties, are discussed.

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Manuscripts available from: cpttrson@tcd.ie

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HIGHLIGHT OF THE MONTH

ON OSCILLATIONS OF THERMODYNAMIC QUANTITIES FOR DEGENERATE FERMI GAS AT LOW TEMPERATURES

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1955 †

Abstract

The electron energy level quantization in a magnetic field leads to oscillations of thermodynamical quatities for the degenerate electron Fermi gas and is the cause of a periodical dependence of the magnetic susceptibility of the electron gas on the magnetic field (de Haas – van Alphen effect). It is obvious that an analogous oscillatory dependence for the degenerate Fermi gas of particles with discrete quantum energy levels on parameters which determine the energy level positions appears always when the quantization of energy levels takes place (for example, bounded volume of the gas or external field with a spatially increasing potential).

It is known that the quantization of energy levels of electrons in a magnetic field leads to oscillations of thermodynamic quantities for a degenerate electron Fermi gas and causes a periodic dependence of magnetic susceptibility of the electron gas on the field strength (de Haas-van Alphen effect) [1]. Obviously, an analogous effect of the oscillating dependence of thermodynamic quantities for a degenerate Fermi gas of particles with quantized energy levels on those parameters which determine the position of these levels will take place always when the causes leading to the quantization of energy levels exist (e. g. finite volume, external fields with an increasing potential, etc.).

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† Originally appeared in the Transactions of the Academy of Sciences of the USSR, Physics Section

Below we calculate the oscillating terms in the thermodynamic potentials causing the whole effect under quite general assumptions regarding the energy spectrum of the particles (or quasiparticles) forming the ideal degenerate Fermi gas.

1 Calculation of oscillating part of thermodynamic potential Ω

Let us suppose that the "classical" problem of the particle motion is solved. Then the energy $\mathcal{E}$ of the particle can be expressed by means of action variables I_i:

$$\mathcal{E} = \mathcal{E}(I_1, I_2, I_3) \tag{1}$$

As the oscillations of thermodynamic quantities at low temperatures are determined by the energy spectrum near the Fermi energy, we shall be interested only in the high energy levels and therefore we can apply the quasiclassical approximation to the quantization of the particle motion. The quasiclassical quantization of a system with several degrees of freedom performing finite motion is given by [2]:

$$I_i = (n_i + \gamma_i)h_i \ ; \qquad\qquad 0 < \gamma_i < 1 \ , \tag{2}$$

and the quantized energy levels E are obtained from (1) by substitution of $(n_i + \gamma_i)h$ for I_i:

$$E(\mathbf{n}) = \mathrm{E}\left[(n_1 + \gamma_1)h,\ (n_2 + \gamma_2)h,\ (n_3 + \gamma_3)h\right]$$

(here $\mathbf{n}$ means a vector with integer components n_1, n_2, n_3).

The thermodynamic potential Ω relevant for the calculation of thermodynamic quantities is given by

$$\Omega = -\theta \sum_{\mathbf{n}} \ln\left\{1 + e^{[\zeta - E(\mathbf{n})]/\theta}\right\},$$

where $\theta = kT$, ζ denotes the chemical potential and the sum extends over all possible values of $\mathbf{n}$.

To get the oscillating part of Ω we use a three-dimensional analogy of Poisson formula where the sum over $\mathbf{n}$ is replaced by the integral:

$$\begin{aligned}\Omega &= \int f[\zeta - E(\mathbf{n})]d\mathbf{n} + 2\mathrm{Re}\sum_{\mathbf{k}} \mathcal{L}_{\mathbf{k}} = \\ &= \frac{1}{h^2}\int f[\zeta - \mathcal{E}(I_1, I_2, I_3)]dI_1 dI_2 dI_3 + 2\mathrm{Re}\sum_{\mathbf{k}} \mathcal{L}_{\mathbf{k}},\end{aligned} \tag{3}$$

where

$$f(x) = -\theta \ln(1 + e^{x/\theta})$$

The vector $\mathbf{k}$ denotes a triplet of integer indices k_1, k_2, k_3 and the sum over $\mathbf{k}$ extends over all non-negative k_1, k_2, k_3 excluding $\mathbf{k} = 0$. The symbol $\mathcal{L}_{\mathbf{k}}$ stands for the following integral:

$$\mathcal{L}_{\mathbf{k}} = \int f([\zeta - E(\mathbf{n})]e^{2\pi\imath\mathbf{kn}}d\mathbf{n}.$$

The oscillating part of Ω is contained in the second term of the expression (3).

Before we calculate the integrals $\mathcal{L}_{\mathbf{k}}$ entering Eq. (3) we note that the integration over $\mathbf{n}$ is carried out only over the first octant (from $n_i = 0$ to $n_i = \infty$). As a consequence and due to the discontinuity of the integrand at the boundary of the region of integration, the result will contain two-dimensional and one-dimensional integrals besides the three-dimensional integrals $\mathcal{L}_{\mathbf{k}}$. Hence, the formula for the oscillating part of Ω reads:

$$\begin{aligned}\Omega_{\mathrm{OSC}} &= 2\mathrm{Re}\sum_{\mathbf{k}}\mathcal{L}_{\mathbf{k}} + \mathrm{Re}\left\{\sum_{k_1,k_2}{}^{'} P_{k_1,k_2} + \sum_{k_1,k_3}{}^{'} P_{k_1,k_3} + \sum_{k_2,k_3}{}^{'} P_{k_2,k_3}\right\} + \\ &+ \frac{1}{2}\mathrm{Re}\left\{\sum_{k_1}{}^{'} Q_{k_1} + \sum_{k_2}{}^{'} Q_{k_2} + \sum_{k_3}{}^{'} Q_{k_3}\right\},\end{aligned} \tag{4}$$

where the two-dimensional integral P_{k_1,k_2} is given by :

$$P_{k_1,k_2} = \int\int f[\zeta - E(n_1, n_2, 0)]e^{2\pi\imath(k_1n_1+k_2n_2)}dn_1dn_2,$$

P_{k_1,k_3} and P_{k_2,k_3} are given by analogy. The one-dimensional integrals Q_{k_1}, Q_{k_2}, Q_{k_3} are given by expressions of the form

$$Q_{k_1} = \int f[\zeta - E(n_1, 0, 0)]e^{2\pi\imath k_1n_1}dn_1$$

Primes at the sum symbols in Eq. (4) means that the term with $\mathbf{k} = 0$ ($k_1 = k_2 = k_3 = 0$) is excluded.

Obviously, the integral $\mathcal{L}_{\mathbf{k}}$ can be transformed to

$$\mathcal{L}_{\mathbf{k}} = \int f(\zeta - E)\left\{\int\limits_{\substack{E(\mathbf{n}) = E \\ n_i \geq 0}} \frac{e^{2\pi\imath\mathbf{kn}}d\Omega_{\mathbf{n}}}{|\nabla E(\mathbf{n})|}\right\}dE,$$

where $d\Omega_{\mathbf{n}}$ denotes an element of the constant energy surface

$$E(\mathbf{n}) = E, \tag{5}$$

in the direction $\mathbf{n}$. The integration in the surface integral inside the braces is restricted to that part of the constant energy surface (5) which lies in the first octant.

Employing the starting assumption regarding the large quantum numbers ($\mathbf{kn} \gg 1$), an asymptotic estimate of the integral $\mathcal{L}_{\mathbf{k}}$ can be obtained [3]:

$$\mathcal{L}_{\mathbf{k}} \approx \int dE f(\zeta - E)\sum_{\nu}\frac{e^{2\pi\imath\mathbf{kn}_\nu \pm\imath\pi/4\pm\imath\pi/4}}{\mid\mathbf{k}\mid\mid\nabla E(\mathbf{n}_\nu)\mid\sqrt{\mid K_\nu(E)\mid}};$$

where $\mathbf{n}_\nu = \mathbf{n}_\nu(\mathbf{k}, E)$ denotes the radius vector in the space $\mathbf{n}$ of those points on the surface (5) at which the direction of the surface normal is paralell to $\mathbf{k}$; $K_\nu(E)$ is the Gaussian curvature of the surface at these points. The sum extends over all such points in the first octant. The phases $\imath\pi/4$ enter the argument of the exponential with the same sign if the point $\mathbf{n}_\nu$ is elliptical. They enter with minus sign if the convexity of the surface at a given point is directed along $\mathbf{k}$ and they enter with plus sign if the convexity is directed in the opposite direction. In case of a hyperbolic point the phases $\imath\pi/4$ enter the exponent with different signs.

Assuming $\partial n_\nu/\partial E \neq 0$ and an obvious condition $\theta \ll \zeta$ the main contribution to the oscillating part of $\mathcal{L}_\mathbf{k}$ comes from integration over the neighbourhood of the sharp non-stationarity of the Fermi distribution function df/dE, i. e. near $E = \zeta$. Taking this into account, we expand $\mathbf{n}_\nu(\mathbf{k}, E)$ in the argument of exponential into powers of $E - \zeta$ and integrate:

$$(\mathcal{L}_\mathbf{k})\mathrm{osc} \approx \frac{1}{(2\pi)^2\sqrt{k_1^2+k_2^2+k_3^2}} \sum_\nu \frac{\Psi(\lambda_\mathbf{k}) e^{2\pi\imath\mathbf{k}\mathbf{n}_\nu(k,\zeta)\pm\imath\pi/4\pm\imath\pi/4}}{(\mathbf{k}, \partial n_\nu/\partial\zeta)^2 \mid \nabla E(\mathbf{n}_\nu) \mid \sqrt{\mid K_\nu(\zeta) \mid}},$$

$$\Psi(\lambda) = \lambda/\sinh\lambda \ ; \qquad \lambda_\mathbf{k} = 2\pi^2(\mathbf{k}, \partial\mathbf{n}_\nu/\partial\zeta)\theta$$

The two-dimensional and one-dimensional integrals can be evaluated similarly. The final results are:

$$(P_{k_1,k_2})\mathrm{osc} \approx \frac{1}{(2\pi)^2(k_1^2+k_2^2)^{\frac{1}{4}}} \times$$

$$\times \sum_\mu \frac{\Psi(\lambda_{k_1,k_2}) e^{2\pi\imath(k_1 n_{\mu 1} + k_2 n_{\mu 2})\pm\imath\pi/4}}{\left(k_1\frac{\partial n_{\mu 1}}{\partial\zeta} + k_2\frac{\partial n_{\mu 2}}{\partial\zeta}\right)^2 \left[\left(\frac{\partial E}{\partial n_1}\right)^2 + \left(\frac{\partial E}{\partial n_2}\right)^2\right]^{\frac{1}{2}} \sqrt{\mid K_{12\mu}(\zeta) \mid}};$$

$$\lambda_{k_1,k_2} = 2\pi^2\theta\left(k_1\frac{\partial n_{\mu 1}}{\partial\zeta} + k_2\frac{\partial n_{\mu 2}}{\partial\zeta}\right);$$

here $n_{\mu i}(\zeta) = n_{\mu i}(k_1, k_2, \zeta)$ denotes the coordinates of those points on the plain curve

$$E(n_1, n_2, 0) = \zeta \tag{6}$$

at which the direction of the curve normal is paralell to the two-dimensional vector (k_1, k_2); $K_{12\mu}(\zeta)$ stands for the curvature of the curve (6) at these points and the sum extends over all such points in the first quadrant. The phase $\imath\pi/4$ enters the exponential with minus sign if the curvature of the curve (6) at the point $(n_{\mu 1}, n_{\mu 2})$ is directed along (k_1, k_2) and it enters with plus sign if the curvature of the curve is in the opposite direction. Further:

$$\begin{aligned}(Q_{k_1})\mathrm{osc} &\approx \frac{\Psi(\lambda_{k_1})}{(2\pi k)^2 \partial n_1/\partial\zeta} e^{2\pi\imath k_1 n_1(\zeta)};\\ \lambda_{k_1} &= 2\pi^2\theta(k_1\frac{\partial n_1}{\partial\zeta});\end{aligned}$$

where $n_1(\zeta)$ denotes this value of n_1 for which $E(n_1, 0, 0) = \zeta$. The formulas for P_{k_1,k_3}, P_{k_3,k_2} and Q_{k_2}, Q_{k_3} have an analogous form. Employing the obtained asymptotic expressions for $\mathcal{L}_{\mathbf{k}}$, P and Q in (4) we get the oscillating part of Ω. It comes out that Ω_{OSC} containes several terms, each of them having its own period of oscillations. The periods of oscillations in individual terms of Ω_{OSC} can be determined from the knowledge of the dependence of the arguments of the corresponding exponentials on the parameters determining the position of energy levels. It should be noted that if the ratio of periods of different terms can be in general arbitrary, the oscillations can have a very complicated form in case of several terms of the same order of magnitude in (4).

The solution of the "classical" problem to find the energy of a particle in the form (1) is connected in general with well-known difficulties and can be performed easily only for separating variables.

We shall give the simplest examples in which it is possible to calculate the oscillating part of the thermodynamic potentials to the very end and to obtain the periods of corresponding oscillations.

2 Electron gas in three-dimensional potential well

Let us consider the electron gas with an arbitrary law of dispersion:

$$\mathcal{E} = \mathcal{E}(p_1, p_2, p_3) \tag{7}$$

in an infinitely high rectangular potential well with sizes L_1, L_2 and L_3 along the respective axes. As it is well-known, the formula (2) in this case reads

$$2p_i L_i = n_i h,$$

and therefore, the quantized energy levels have the form:

$$\mathcal{E}(\mathbf{n}) = \mathcal{E}\left(\frac{n_1 h}{2L_1}, \frac{n_2 h}{2L_2}, \frac{n_3 h}{2L_3}\right) \tag{8}$$

Performing the calculation according to the formulas of section 1 using (8) it is possible to get all terms of the oscillating part of the thermodynamic potential Ω (because of the two possibleelectron spin orientations, the right-hand side of the formula for Ω must be additionally multiplied by 2). It turns out that if we exclude the anomalously high anisotropy of the boundary surface $\mathcal{E}(\mathbf{p}) = \zeta$ then for $L_1 \approx L_2 \approx L_3 = L$ we can write

$$\frac{\mathcal{L}_{\mathbf{k}}}{P} \approx \frac{P}{Q} \approx \frac{L^{1/2}}{\left(\frac{h\partial^2\mathcal{E}/\partial p^2}{\partial\mathcal{E}/\partial p}\right)^{1/2}}$$

where the quantity $\frac{h\partial^2\mathcal{E}/\partial p^2}{\partial\mathcal{E}/\partial p}$ is equal to the de Broglie wavelenght of an electron λ_B.

Considering $L \gg \lambda_B$ we can leave in the expression for (4) only the terms containing Ω_{osc} Then

$$\Omega_{\mathrm{osc}} = \Omega_1 + \Omega_2 + \Omega_3. \tag{9}$$

Here

$$\begin{aligned}\Omega_1 &= L_1 L_2 L_3 \frac{1}{\pi^2}\left\{\sum_{\nu}\sum_{k_1=1}^{\infty} \beta^2(\mathbf{k}) \frac{\Psi(\lambda_{\mathbf{k}}) \cos(2\pi k_1 n_{\nu 1} \pm \pi/4 \pm \pi/4)}{\sqrt{\mid D(k_1,0,0) \mid}} + \right.\\ &+ \left. \sum_{\nu'}\sum_{k_2=1}^{\infty} \cdots + \sum_{\nu''}\sum_{k_3=1}^{\infty} \cdots \right\}.\end{aligned}$$

The dots in the last two sums stand for expressions analogous to that one in the first sum; $\mathbf{n}_\nu(k_1)$ is the radius vector of a point of the boundary surface $E(\mathbf{n}) = \zeta$, at which the surface normal is paralell to the vector $(k_1, 0, 0)$. The vectors $\mathbf{n}(k_2)$ and $\mathbf{n}(k_3)$ and are defined in analogy.

$$\begin{aligned}\Omega_2 &= L_1 L_2 L_3 \frac{1}{\pi^2}\left\{\sum_{\mu}\sum_{k_1 k_2=1}^{\infty} \beta^2(\mathbf{k}) \frac{\Psi(\lambda_{\mathbf{k}}) \cos(2\pi k_1 n_{\mu 1} + k_2 n_{\mu 2} \pm \pi/4 \pm \pi/4)}{\sqrt{\mid D(k_1,k_2,0) \mid}} + \right.\\ &+ \left. \sum_{\mu'}\sum_{k_1 k_3=1}^{\infty} \cdots + \sum_{\mu''}\sum_{k_2 k_3=1}^{\infty} \cdots \right\},\end{aligned}$$

where $\mathbf{n}_\mu(k_1, k_2)$ is the radius vector of a point at which the normal to the boundary surface $E(\mathbf{n}) = \zeta$ is paralell to the vector $(k_1, k_2, 0)$. The vectors $\mathbf{n}_{\mu'}(k_1, k_3)$ and $\mathbf{n}_{\mu''}(k_2, k_3)$ are defined in analogy.

$$\Omega_3 = L_1 L_2 L_3 \frac{1}{(3\pi)^2} \sum_{\rho} \sum_{k_1 k_2 k_3=1}^{\infty} \beta^2(\mathbf{k}) \frac{\Psi(3\lambda_{\mathbf{k}}) \cos(2\pi \mathbf{k}\mathbf{n}_\rho \pm \pi/4 \pm \pi/4)}{\sqrt{\mid D(k_1,k_2,k_3) \mid}},$$

where $\mathbf{n}_\rho(k_1, k_2, k_3)$ is the radius vector of a point at which the normal to the boundary surface is paralell to the vector $\mathbf{k}$:

$$\lambda_{\mathbf{k}} = \frac{(2\pi)^2 \theta}{h\beta(\mathbf{k})};$$

$$D(k_1,k_2,k_3) = \begin{vmatrix} \partial^2\mathcal{E}/\partial p_1^2 & \partial^2\mathcal{E}/\partial p_1 \partial p_2 & \partial^2\mathcal{E}/\partial p_1 \partial p_3 & K_1 L_1 \\ \partial^2\mathcal{E}/\partial p_1 \partial p_2 & \partial^2\mathcal{E}/\partial p_2^2 & \partial^2\mathcal{E}/\partial p_2 \partial p_3 & k_2 L_2 \\ \partial^2\mathcal{E}/\partial p_1 p_3 & \partial^2\mathcal{E}/\partial p_2 \partial p_3 & \partial^2\mathcal{E}/\partial p_3^2 & k_3 L_3 \\ k_1 L_1 & k_2 L_2 & k_3 L_3 & 0 \end{vmatrix}.$$

The values of $\lambda_{\mathbf{k}}$ and $D(k_1, k_2, k_3)$ are taken at the corresponding points on the boundary surface.

The symbol $\beta(\mathbf{k})$ was used to denote the expressions

$$\frac{\partial\mathcal{E}/\partial p_1}{k_1 L_1} = \frac{\partial\mathcal{E}/\partial p_2}{k_2 L_2} = \frac{\partial\mathcal{E}/\partial p_3}{k_3 L_3} \beta(\mathbf{k}) \tag{10}$$

taken at the same points. Assuming $L_3 \gg L_1 \approx L_2$ the formula (9) for Ω_{osc} can be simplified. In the case of infinitely large L_3, it follows from Eq. (10) that $k_3 = 0$ and hence Ω_3 in (9) vanishes and in the formulas for Ω_1 and Ω_2 only the terms with sums over k_1 and k_2 survive.

Finally, assuming $L_2 \approx L_3 \gg L_1$, i. e. in case of an electron gas confined between two infinitely high walls we get

$$\begin{aligned} \Omega_{\mathrm{osc}} &= \Omega_1 = \\ &= \frac{L_2 L_3}{L_1^2}\frac{1}{\pi^2}\sum_{\nu}\sum_{k=1}^{\infty}\frac{(\partial\mathcal{E}/\partial p_1)^2\Psi\left(\frac{4\pi^2 k L_1\theta}{h\partial\mathcal{E}/\partial p_1}\right)}{\left|\frac{\partial^2\mathcal{E}}{\partial p_2^2}\frac{\partial^2\mathcal{E}}{\partial p_3^2}-\left(\frac{\partial^2\mathcal{E}}{\partial p_2\partial p_3}\right)^2\right|^{\frac{1}{2}}}\cos(2\pi k n_{\nu_1}\pm\frac{\pi}{4}\pm\frac{\pi}{4}) \end{aligned} \qquad (11)$$

The formulas given above for the oscillating part of Ω take the simplest form in case of an electron gas with a quadratic dispersion law

$$\mathcal{E} = \frac{p^2}{2m} \equiv \frac{p_x^2 + p_y^2 + p_z^2}{2m}$$

placed in a cubic potential well

$$(L_1 = L_2 = L_3 = L).$$

In this case the terms entering (9) have the form

$$\begin{aligned} \Omega_1 &= \frac{6\zeta}{\pi^2}\sum_{k=1}^{\infty}\frac{1}{k^3}\Psi\left(2\sqrt{2}\pi^2 k\frac{\sqrt{m}\theta L}{h\sqrt{\zeta}}\right)\sin\left(4\pi k L\frac{\sqrt{2m\zeta}}{h}\right); \\ \Omega_2 &= \frac{6\zeta}{(2\pi)^2}\sum_{k_1,k_2=1}^{\infty}\frac{1}{(k_1^2+k_2^2)^{3/2}}\Psi\left(4\sqrt{2}\pi^2\sqrt{k_1^2+k_2^2}\frac{\sqrt{m}\theta L}{h\sqrt{\zeta}}\right)\times \\ &\quad \times\sin\left(4\pi\sqrt{k_1^2+k_2^2}L\frac{\sqrt{2m\zeta}}{h}\right); \\ \Omega_3 &= \frac{2\zeta}{(3\pi)^2}\sum_{k_1,k_2,k_3=1}^{\infty}\frac{1}{\mid\mathbf{k}\mid^3}\Psi\left(6\sqrt{2}\pi^2\mid\mathbf{k}\mid\frac{\sqrt{m}\theta L}{h\sqrt{\zeta}}\right)\times \\ &\quad \times\sin\left(4\pi\mid\mathbf{k}\mid L\frac{\sqrt{2m\zeta}}{h}\right). \end{aligned}$$

If the temperature of the gas is very low or if the size of the potential well is very small, so that $\lambda_{\mathbf{k}} \equiv 2\sqrt{2}\pi^2\frac{\sqrt{m}\Theta L}{h\sqrt{\zeta}} \ll 1$, the function $\Psi(\lambda_{\mathbf{k}})$ can be replaced by unity. If the size of the potential well is large and $\lambda_{\mathbf{k}} \gg 1$, then $\Psi(\lambda_{\mathbf{k}}) \approx 2\lambda_{\mathbf{k}}e^{-\lambda_{\mathbf{k}}}$ and in formula (9) only the first term of the sum for Ω_1 survives.

$$\Omega_{\mathrm{osc}} \approx 24\theta L\frac{\sqrt{2m\zeta}}{h}\exp\left\{-2\sqrt{2}\pi^2\frac{\sqrt{m}\theta L}{h\sqrt{\zeta}}\right\}\sin\left(4\pi L\frac{\sqrt{2m\zeta}}{h}\right).$$

It can be seen from the last expression that the variation of the linear size of the potential well leads to the oscillations of the thermodynamic potential Ω with the period

$$\Delta L = \frac{h}{2\sqrt{2m\zeta}}$$

which does not depend on L. Note that this period is identical with the half length of de Broglie wave for electrons at the boundary surface. As the number of the de Broglie halfwaves, $h/2\sqrt{2m\zeta}$, which can be placed between the potential walls determines the index of a boundary stationary state, each "vibration" of Ω is connected with a unit change of the number of levels lying below the boundary energy.

3 Electron gas in potential well in magnetic field

Consider the electron gas with an arbitrary dispersion law (7) in the same potential well as in section 2 placed in a homogenous magnetic field $\mathbf{H}$ applied along the x_3 axis. If we choose the vector potential in the form $A_1 = -Hx_2$, $A_2 = A_3 = 0$, two of the conditions (2) are reduced to obvious relations:

$$2p_1L_1 = n_1h, \quad 2p_3L_3 = n_3h.$$

The third condition can be written in the form [4]:

$$S\left(E, \frac{n_1h}{2L_1}, \frac{n_3h}{2L_3}; H\right) = (n_2 + \gamma)\frac{ehH}{c}, \tag{12}$$

where $S(E, p_x, p_z; H)$ is the area of the intersection of the constant energy surface

$$\mathcal{E}(P_1, P_2, P_3) = E, \;\; p_x - \frac{|e|H}{c}\frac{L_2}{2} < P_1 < p_x + \frac{|e|H}{c}\frac{L_2}{2}$$

by the plane $P_3 = p_z = \text{const}$.

The energy levels E are given by expression following from (12):

$$E = E(n_1, n_2, n_3; H).$$

If L_2 is small, one can suppose that the mean diameter of the classical electron orbit in the magnetic field is grater than L_2. In such case, E is determined by different analytical expressions according to the relations between the diameter of the curve $\mathcal{E}(P_1, P_2, p_z) = E$, $p_z = \frac{n_3h}{2L_3} = \text{const.}$ and the quantity $\left|\frac{n_1h}{L_1} \pm \frac{eH}{c}L_2\right|$.

Employing (12) and performing the calculations according to the formulas of section 1 (taking into account the electron spin) we obtain all terms of the oscillating part of the thermodynamic potential Ω. A comparison of terms containing $\mathcal{L}_{\mathbf{k}}$, P and Q shows that for $L_1 \approx L_3 = L$ their ratio is equal to :

$$\frac{\mathcal{L}_{\mathbf{k}}}{P} \approx \frac{P}{Q} \approx \frac{\gamma L}{(ch/eH)^{1/2}},$$

where the quantity $(ch/eH)^{1/2}$ has a simple physical meaning: it is identical to the radius of the classical electron orbit in the magnetic field $r_0(H)$ corresponding to the lowest energy level ($n_2 = 0$). Really, as for small p one can always use the quadratic expansion of the expression (7), the lowest energy levels of the electron motion in the magnetic field are of the form: $E_{n_2} = \left(n_2 + \frac{1}{2}\right)\frac{ehH}{m^\star c}$ where $m^\star$ is an effective mass, and therefore

$$r_0(H) = \frac{c\sqrt{2m^\star E_0}}{eH} = \left(\frac{ch}{eH}\right)^{1/2}.$$

Assuming $L \gg r_0(H)$, we can leave as in 2 only those terms of Ω_{osc} which contain $\mathcal{L}_{\mathbf{k}}$:

$$\Omega_{\text{osc}} = \Omega^{(1)} + \Omega^{(2)} + \Omega^{(3)}$$

here

$$\Omega^{(1)} = L_1 L_3 \left(\frac{eH}{c}\right)^2 \frac{4}{\pi^2} \sum_m \sum_{k_2=1}^{\infty} \frac{\Psi(\lambda_{k_2}) \cos\left[\frac{2\pi k_2 c S_m(H)}{ehH} \pm \frac{\pi}{4} \pm \frac{\pi}{4} - 2\pi k_2 \gamma\right]}{k_2^3 \Phi(\zeta, \mathbf{n}_m)},$$

where $\mathbf{n}_m(H)$ is the radius vector of a point at which $S(\zeta, p_x, p_z; H)$ has an extremal value $S_m(H)$ at constant ζ : $\left.\frac{\partial S}{\partial p_x}\right|_m = \left.\frac{\partial S}{\partial p_z}\right|_m = 0$; the normal to the surface

$$E(n_1, n_2, n_3; H) = \zeta \tag{13}$$

at this point is paralel to axis n_2;

$$\begin{aligned} \Omega^{(2)} &= L_1 L_3 \left(\frac{eH}{c}\right)^2 \frac{1}{\pi^2} \left\{ \sum_\mu \sum_{k_2=1}^{\infty} \frac{1}{k_2^3} \sum_{k_1=1}^{\infty} \frac{\Psi(2\lambda_{k_2}) \cos\left[2\pi(k_1 n_{\mu 1} + k_2 n_{\mu 2}) \pm \frac{\pi}{4} \pm \frac{\pi}{4}\right]}{\Phi\left[\zeta, \mathbf{n}_\mu(k_1, k_2)\right]} + \right. \\ &+ \left. \sum_{\mu'} \sum_{k_2=1}^{\infty} \frac{1}{k_2^3} \sum_{k_3=1}^{\infty} \frac{\Psi(2\lambda_{k_2}) \cos\left[2\pi(k_3 n_{\mu' 3} + k_2 n_{\mu' 2}) \pm \frac{\pi}{4} \pm \frac{\pi}{4}\right]}{\Phi\left[\zeta, \mathbf{n}_{\mu'}(k_3, k_2)\right]} \right\};\end{aligned}$$

where $\mathbf{n}_\mu(k_1, k_2, H)$ is the radius vector of a point at which the normal to the surface (13) is paralell to the vector $(k_1, k_2, 0)$ and $\mathbf{n}_{\mu'}(k_3, k_2, H)$ is defined analogously;

$$\Omega^{(3)} = L_1 L_3 \left(\frac{eH}{c}\right)^2 \left(\frac{2}{3\pi}\right)^2 \sum_\rho \sum_{k_2=1}^{\infty} \frac{1}{k_2^3} \sum_{k_1, k_3=1}^{\infty} \frac{\Psi(3\lambda_{k_2}) \cos\left[2\pi \mathbf{k}\mathbf{n}_\rho(\mathbf{k}) \pm \frac{\pi}{4} \pm \frac{\pi}{4}\right]}{\Phi\left[\zeta, \mathbf{n}_\rho(\mathbf{k})\right]}$$

where $\mathbf{n}_\rho(\mathbf{k}, H)$ is the radius vector of a point at which the normal to the surface (13) is paralell to the vector $\mathbf{k}$;

$$\lambda_{k_2} = 2\pi^2 k_2 \frac{c\theta}{ehH}\left(\frac{\partial S}{\partial \zeta}\right), \quad \Phi(\zeta, \mathbf{n}) = \left|\frac{\partial S}{\partial \zeta}\right| \left|\frac{\partial^2 S}{\partial p_x^2}\frac{\partial^2 S}{\partial p_z^2} - \left(\frac{\partial^2 S}{\partial p_x \partial p_z}\right)^2\right|^{1/2}$$

The values λ_{k_2} and $\Phi(\zeta, \mathbf{n})$ are taken at the corresponding points.

It should be noted that if some of the enumerated points lies in the coordination plane of the **n**-space, the corresponding term must be multiplied by $\frac{1}{2}$; if this point lies in one of the coordination axes, it is necessary to multiply the corresponding term by $\frac{1}{4}$.

The formula for Ω_{osc} simplifies in two limiting cases: If $\lambda_{k_2} \ll 1$ then the function $\Psi(\lambda_{k_2})$ can be replaced by unity; if the $\lambda_{k_2} \gg 1$, then $\Psi(\lambda_{k_2}) \approx 2\lambda_{k_2} e^{-\lambda_{k_2}}$ and therefore only the first terms remain in the sums over $\mathbf{k}$. The last case corresponds to a strengthened inequality

$$\frac{c\theta}{ehH}\left(\frac{\partial S}{\partial \zeta}\right) \gg 1 \tag{14}$$

which has a simple physical meaning. As follows from (12), the mean distance between neighbouring energy levels with quantum numbers n_2 and n_2+1 near the boundary energy is given by

$$\Delta E_{n_2} = \frac{\frac{ehH}{c}}{\frac{\partial S}{\partial \zeta}}$$

and therefore the inequality (14) corresponds to

$$\zeta \gg \theta \gg \Delta E_{n_2}$$

If this inequality is fulfilled, Ω_{osc} consists of terms of the form

$$\Omega_{\mathrm{osc}} \sim B(L_1, L_2, L_3; H, \zeta) \cos\left[2\pi n(L_1, L_2, L_3; H, \zeta) \pm \pi/4 \pm \pi/4\right]$$

The amplitude of the oscillations B and their phases $2\pi n$ have for $\Omega^{(j)}$ $(j = 1, 2, 3)$ the following forms:

$$\begin{array}{rcll}
B(L_1, L_2, L_3; H, \zeta) & = & L_1 L_2 \frac{16}{j} \frac{eH\theta}{ch} \left(\frac{\partial S}{\partial \zeta}\right) \frac{\exp\left\{-j2\pi^2 \frac{c\theta}{ehH} \frac{\partial S}{\partial \zeta}\right\}}{\Phi(\zeta, \mathbf{n})} & (j = 1, 2, 3) \\
n & = & \frac{cS_m(H)}{ehH} - 2\pi\gamma & \text{for } j = 1, \\
n & = & n_{\mu 1}(L_1, L_1, L_3; H, \zeta) + n_{\mu 2}(L_1, L_2, L_3; H, \zeta) & \text{for } j = 2, \\
n & = & n_{\rho 1}(L_1, L_1, L_3; H, \zeta) + & \\
 & & + n_{\rho 2}(L_1, L_1, L_3; H, \zeta) + n_{\rho 3}(L_1, L_1, L_3; H, \zeta) & \text{for } j = 3.
\end{array}$$

The dependence of the phase $2\pi n$ on the intensity of the magnetic field H and on the sizes of the potential well L_1, L_2, L_3 determine the periods of oscillations of Ω_{osc} with changes of these parameters.

It is easy to prove that the oscillation periods of the terms of Ω_{osc} with the changes of H are given by the following formulas:

$$\begin{array}{lllcl}
1) & \text{for } \Omega^{(1)} & \Delta\left(\frac{1}{H}\right) & = & \frac{eh/c}{|S_m(H) - H\partial S_m/\partial H|}, \\
2) & \text{for } \Omega^{(2)} & \Delta\left(\frac{1}{H}\right) & = & \frac{eh/c}{2|S(\mathbf{n}_\mu, H) - H\partial S_\mu/\partial H|}, \\
3) & \text{for } \Omega^{(3)} & \Delta\left(\frac{1}{H}\right) & = & \frac{eh/c}{3|S(\mathbf{n}_\rho, H) - H\partial S_\rho/\partial H|}.
\end{array}$$

In a similar way, it is possible to obtain the periods of oscillations with the changes of L_1, L_2, L_3.

Supposing that $L_3 \gg L_1$ then $k_3 = 0$ and the following formula is valid for Ω_{osc}:

$$\begin{array}{rcl}
\Omega_{\mathrm{osc}} & = & \Omega_1 + L_1 L_2 \left(\frac{eH}{c}\right)^2 \frac{1}{\pi^2} \sum\limits_{\mu} \sum\limits_{k_2=1}^{\infty} \frac{1}{k_2^3} \sum\limits_{k_1=1}^{\infty} \Psi(2\lambda_{k_2}) \times \\
 & \times & \frac{\cos\left[2\pi(k_1 n_{\mu 1} + k_2 n_{\mu 2}) \pm \frac{\pi}{4} \pm \frac{\pi}{4}\right]}{\Phi[\zeta, \mathbf{n}_\mu(k_2, k_3)]}.
\end{array}$$

Finally, assuming that $L_1, L_3 \gg L2$, the formula for Ω_{osc} consists only of the first term (Ω_1):

$$\begin{aligned}\Omega_{\text{osc}} &= \Omega_1 = L_1 L_3 \left(\frac{eH}{c}\right)^2 \frac{4}{\pi^2} \times \\ &\times \sum_m \sum_{k_2=1}^{\infty} \frac{\Psi(\lambda_{k_2}) \cos\left[\frac{2\pi k_2 c S_m(H)}{ehH} \pm \frac{\pi}{4} \pm \frac{\pi}{4} - 2\pi k_2 \gamma\right]}{k_2^3 \Phi(\zeta, \mathbf{n}_m)} \end{aligned} \tag{15}$$

which coincides with the formula derived by the present authors for the case of a one-dimensional infinitely deep potential well [4] in a slightly different way[1] .

It is not difficult to verify that in the limiting case $H \to 0$ the formula (15) transforms in (11).

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[1] In [4] a formula for the oscillating part of the magnetic moment of an electron gas M_{osc} was obtained. Using $M = -\partial\Omega/\partial H$ and employing the fact that the prefactor of cosine in (15) need not be differentiated, it is easy to prove the equivalence of both formulas.