Cezary Śliwa

Summary of academic achievements

Institute of Physics, Polish Academy of Sciences
Warsaw (Poland), 2013

Spis treści

Rozdział 1

Scientific *curriculum vitae*

1.1 Personal and bibliometric data

Name:	Cezary Łukasz Śliwa
H-Index according to ISI WOK:	10
Numer of published papers:	16
Citation count (total):	416
Citation count (no auto-citations):	408
Total Impact Factor:	62.285

Remarks:

- the Impact Factor given above is calculated according to the data for the publication year or the year 2012 for publications earlier than 2007;
- by an auto-citation we mean above a citation in another publication (co)authored by the present candidate.

1.2 Important dates

1991 started studies at the Faculty of Physics, University of Warsaw

1996 master thesis „Standardowe grupy kwantowe jako grupy ilorazowe grup podwojonych" ["Standard quantum groups as the quotients of double groups"]

1996 employment at Centre for Theoretical Physics, Polish Academy of Sciences, Warsaw (as an assistant before 2002, as an assistant professor since 2003)

2002 doctoral dissertation „Metoda elementów skończonych w kwantowej teorii pola" ["Finite element method in quantum field theory"]; PhD in physics awarded by the Faculty of Physics, Uniwersity of Warsaw

2002 a six-month stay at the Centre for Quantum Computation, Oxford (financed by ESF)

2004 employment outside of the academy

2005 employment at the Institute of Physics, Polish Academy of Sciences (as an assistant professor, up to now)

1.3 The course of academic career

My academic carreer started already when I was at high school. As a beneficient of a program of the Polish Children's Fund for talented young students I participated in a workshop on physics which took place at the Institute of Physics, Polish Academy of Sciences. The workshop resulted in a publication on the physics of superconductors, the (chronologically) first item in the listing of publications.

During my master studies the the Faculty of Physics, University of Warsaw, I was involved in the calculation of the matrix elements in a tight binding approximation for a microscopic theory of exchange interactions in PbMnTe and PbEuTe that prof. T. Dietl of the Institute of Physics was developing with his coworkers; this is the (chronologically) second item in the listing; thus, these were already materials closely related to the subject of the publication sequence that comprise the basis of the present habilitation procedure.

I have chosen a specialization in mathematical physics and have finished my master studies at the Chair of Mathematical Methods in Physics, where under the supervision of prof. S. L. Woronowicz I have prepared my master thesis on quantum groups (these are mathematical objects which are more general than groups — well known in classical mathematics).

After I finished the studies I was employed at the Centre for Theoretical Physics, Polish Academy of Sciences, and started working in the field of quantum field theory, particularly on discretized models of quantum fields (on a lattice). My particular interest was the application of the methods known from the theory of Lie group and algebras to define and derive a model of quantum electrodynamics for the case of the electron Dirac field and for the case of a (spinless) scalar particle. The doctoral thesis supervisor was prof. J. Kijowski. I also took part in theoretical studies of quantum vortices that was pursued by Prof. I. Białynicki-Birula and Prof. Z. Białynicka-Birula (these developments find their applications e.g. in transmission electron microscopy).

After I was awarded a PhD I was solving problems related to optical implementations of quantum information processing (such as preparation of entangled states and photon-number-sensitive detection) and those pertaining to Bell inequalities. My results from this time are:

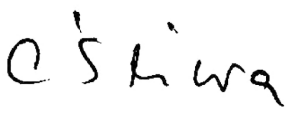
1. the development of a scheme of conditional preparation of pairs of photons in an entangled state, based on a standard parametric down-convertion (PDC) source; in the proposed setup there is one of three pairs of photons (from a standard non-deterministic source) prepared in a maximally entangled state whenever the remaining four photons have been (coincidentally) registered by the "event-ready" detectors; therefore, the coincidence of signals from the "event-ready" detectors heralds the availability of an entangled photon pair at the output of the setup without affecting the prepared state;

2. development of a realistic scheme for detection of photons with resolution of their count; photon-number sensitive detection of light is a prerequisite for schemes such as the one described above, where the detection of exactly one photon guarantees the presence of the remaining photons at the output of the setup; in the proposed detection scheme the signal (a pulse of light) is divided into pulses, separated in time, which are directed onto a pair of standard detectors;

3. discovery of the symmetries of the Bell inequalities; in particular, the derivation of a single new inequality which generates the whole Bell polytope (a full set of Bell inequalities) under the action of the symmetries in the case of $3+3$ observables, and also the classification of all the inequalities for $2+2+2$ observables.

The scheme for preparation of entangled state described above (item 1) has already been realized experimentally.

Since 2005, when I was employed at the Institute of Physics, I work on the physics of ferromagnetic semiconducting compounds, and in particular on the archetypical (Ga,Mn)As. The publications I have coauthored during this time pertain to the magnetic, electronic and thermodynamic properties of this material. **The published results are described in detail in the separate *summary of the sequence of publications comprising the dissertation*.**



Cezary Śliwa

Effective strains in magnetic semiconducting alloys

Summary of results from the sequence of publications comprising the dissertation

Institute of Physics, Polish Academy of Sciences
Warsaw (Poland), 2013

The list of the publications, comprising a sequence and sharing a common subject, submitted as the basis of the habilitation procedure

D1. C. Śliwa, T. Dietl, *Magnitude and crystalline anisotropy of hole magnetization in (Ga,Mn)As*, Phys. Rev. B **74**, 245215, 2006

D2. C. Śliwa, T. Dietl, *Electron-hole contribution to the apparent s-d exchange interaction in III-V dilute magnetic semiconductors*, Phys. Rev. B **78**, 165205, 2008

D3. W. Stefanowicz, C. Śliwa, P. Aleshkevych, T. Dietl, M. Doppe, U. Wurstbauer, W. Wegscheider, D. Weiss, M. Sawicki, *Magnetic anisotropy of epitaxial (Ga,Mn)As on (113)A GaAs*, Phys. Rev. B **81**, 155203, 2010

D4. U. Wurstbauer, C. Śliwa, D. Weiss, T. Dietl, W. Wegscheider, *Hysteretic magnetoresistance and thermal bistability in a magnetic two-dimensional hole system*, Nat. Phys. **6**, 955, 2010

D5. C. Śliwa, T. Dietl, *Thermodynamic and thermoelectric properties of (Ga,Mn)As and related compounds*, Phys. Rev. B **83**, 245210, 2011

D6. M. Birowska, C. Śliwa, J. A. Majewski, T. Dietl, *Origin of bulk uniaxial anisotropy in zinc-blende dilute magnetic semiconductors*, Phys. Rev. Lett. **108**, 237203, 2012

Contents

Chapter 1

Introduction

The common subject of the publications summarized here is the theoretical description of a class of magnetic materials known as the diluted ferromagnetic semiconductors. These are the materials which constitute an alloy of a semiconductor and a magnetic element as the dopant [1]; therefore they enjoy the magnetic properties while preserving the main features of the semiconductor they are based on (the matrix). This unique combination lets us hope to integrate the functionality typical for magnetic materials (storage of information) with the well-founded functionality and technology of semiconductors (computation and information processing). The non-equilibrium growth methods (low-temperature molecular beam epitaxy) made it possible to overcome the limits of the dopant solubility and obtain samples of a diluted material with the composition required for ferromagnetism. Epitaxial layers of the most widely known material from this class, namely the alloy of gallium arsenide (GaAs) and manganese (Mn), exhibit ferromagnetism with the Curie temperature reaching 200 K.

From the point of view of a researcher working in physics, the magnetic dopant in a semiconductor is the system which allows to study the most fundamental laws of nature. It is through the magnetic phenomena that the principles of the relativity theory and quantum mechanics find their manifestation; indeed, the magnetic field is created by a charge in motion, therefore in some systems of units the equations for magnetic effects include the light velocity c, and according to the well-known Bohr-van Leeuwen theorem the classical physics does not admit para-, dia- or ferromagnetism. The elementary object we consider in the theory of magnetism is an electron spin, theoretically described by the relativistic and quantum Dirac equation.

In the case of diluted ferromagnetic semiconductors we consider two kinds of spins: the spins of the electrons partly occupying the orbitals of the magnetic dopants (the local spins), and the spins of the carriers which are present in the conduction or valence band of the semiconductor matrix. In (Ga,Mn)As — the material we study here — the magnetic dopant is a single acceptor, therefore we expect the presence of holes, with the concentration approaching that of the dopant. In the presently accepted model [2] we consider the exchange interaction between the local spins and the band carriers, which leads to the emergence of spontaneous magnetization (ferromagnetism).

As a comment which is in order here, we note that some authors believe that the holes in (Ga,Mn)As ocuppy the states in a hypothetical impurity band above the valence band [3]. As we will see later, in view of the theoretical results published in the sequence, the impurity-band hypothesis does not survive a confrontation with experimental data.

The known magnetic materials differ in their features such as the critical temperature of the ferromagnetic transition (the Curie temperature), the magnitude of the spontaneous magnetization as the function of temperature, magnetic anisotropy (the dependence of the free energy of the system, subject to an external magnetic field, on the resulting direction of magnetization). In the case of (Ga,Mn)As and similar materials, many of these characteristics follow from the known properties of the band carriers. Under the assumption that these properties are grossly unmodified with respect to the matrix, the experimentally available properties of the diluted magnetic material can be predicted.

The first of the publications in the sequence (D1) presents the results obtained according to the above guidelines for the carrier contribution to the total magnetization, taking into account the anisotropy of the valence band. As a necessary prerequisite, the effect of external magnetic field on the holes' orbital degrees of freedom was included without any further approximations (usually, this effect is included at the level of a spherical or axial approximation, or neglected altogether due to resulting numerical complexity). The method employed was to proceed through direct diagonalization of the Hamiltonian, equivalent to solving the Schrödinger equation for the Landau levels in magnetic field of any direction (relative to the crystal principal directions).

The purpose of the next publication in the sequence (D2) is to explain the result of an experiment which indicates that the spin splitting of photoelectrons in (Ga,Mn)As, which quantifies the value of the s–d exchange constant, has an unusual value for the material class in question. The explanation assumes that, under the conditions of the experiment, the photoelectrons do not interact with a free acceptor, but rather with a complex consisting of an acceptor and the acceptor bound hole. The constant that characterizes the exchange interaction between the photoelectron and such a complex has been expressed in terms of the exchange splitting in the neutral exciton, which is known from earlier experiments. The resulting theoretical description is fully consistent with the experiment.

Before proceeding to the next item from the listing of the sequence let us make a general remark. One of the most important mathematical tools in physics, and particularly in solid state physics, is the group theory. In its typical application it allows to predict, from the known symetries of an idealized crystal, the symetries of the interactions, from which the symmetries of the material properties follow. One can say, thus, that the symmetry of the observed material properties reflects the nature of their source, and therefore becomes a qualitative characteristic of the material. This makes it possible to infer the unknown symmetry of the material system from the symmetries of its observed properties (e.g., the symmetry of a crystal lattice can be obtained from x-ray diffraction data) or the existence of a previously unknown interaction (if the observed symmetry deviates from expectations).

In the case of (Ga,Mn)As such a deviation between the expected and observed symmetry became clear not much later than the first epitaxial layers of this material were obtained. The lattice directions [110] and $[\bar{1}10]$ are manifestly inequivalent, despite they transform

one into another under the rotations about the twofold axes [100] and [010] [such rotations preserve the layer plane (001)]. This feature is known as the [110] uniaxial, in-plane uniaxial, or — simply — uniaxial anisotropy, and its presence is the basis of applications such as magnetization direction switching controlled by means of an electrical gate. As an attempt to explain or describe this component of anisotropy, earlier works introduced into the theory some additional deformation (strain), which however has not been observed in x-ray diffraction. Therefore the magnitude of this additional strain should be considered a phenomenological parameter.

The subject of the publication designated as (D3) are the magnetic properties of (Ga,Mn)As layers which are grown on substrates of the non-standard [113] orientation. They differ from the routinely obtained layers in the form of the strain introduced by the lattice mismatch. For a general orientation of the substrate this form becomes a complicated function of the elastic constants of the material. The theoretical part of the publication compares experimental results for magnetic anisotropy in such layers with the predictions of the theory. It has been shown that the observed magnetic anisotropy can be reproduced in the theoretical description assuming that the additional strain which breaks the expected symmetry has only components which are off-diagonal in the coordinate system corresponding to the crystal principal axes (except for the cubic component, which is of higher order, however). The form of the additional off-diagonal strain differs in relation to the layers of the standard (001) orientation which were studied earlier.

The origin of the [110] uniaxial anisotropy has become the subject of publication (D6). According to the point of view presented therein, since the diluted magnetic material is an alloy, it is not justified to assume the symmetry of an ideal crystal. The starting point of the publication is the hypothesis that the presence of the additional anisotropy component can be attributed to a non-random spatial distribution of the magnetic dopant at the sub-nanometer scale, beyond the range available to current characterization methods. The approach that has been developed justifies the description of the resulting magnetic anisotropy in terms of effective strains and allows to predict the magnitude of its components, providing strong support to the validity of the initial hypothesis.

The concern of publication (D5) are the thermodynamic and thermoelectric properties of (Ga,Mn)As. In (D5), the Gaussian approximation to the distribution of the thermal fluctuations has allowed to describe the quantities which are not available to the standard mean field theory, namely the critical behavior of the specific heat. The Seebeck coefficient (the thermopower) has been calculated separately for the heavy and light-hole bands as a function of the total hole concentration. The theoretical predictions, confronted with experimental data, confirm the hypothesis that the electronic properties of (Ga,Mn)As, and the density of states at the Fermi level in particular, remain unchanged with respect to GaAs

In contrast with the other items from the list, publication (D4) is not devoted to (Ga,Mn)As, buth rather to quantum wells of another III-V material, namely InAs. In the theoretical part, the bistability and hystereses that are observed in the experimental setup in external magnetic field are explained. According to the presented theory, built upon an acceptor model similar to that from (D2) and a thermal model of the system, the experi-

mental results of the publication reflect the interplay of two kinds of bistability: a magnetic one, resulting from the strong exchange coupling of the hole's and Mn dopant's spins, and a thermal one, resulting from the thermal balance in the presence of a strong dependence of the resistivity on the magnetization. This shows that the long-range ferromagnetic order is not necessary for magnetic hysteresis to emerge.

Chapter 2

Assumptions underlying the model

According to the remarks in the introduction, the starting point of the sequence of publications is the model of the band structure of the semiconductor matrix, derived from the symmetry of the crystal lattice (i.e. the six-band $\mathbf{k} \cdot \mathbf{p}$ model of the valence band in the zinc-blende structure and a simple forbidden gap at the Γ point), taking into account as a perturbation the macroscopic deformation — through the Pikus-Bir Hamiltonian, and — through the Peierls substitution ($\mathbf{p} \to \mathbf{p} + e\mathbf{A}$) — the effect of an external magnetic field.

In the case of a manganese dopant in GaAs, the total orbital angular momentum of the electrons occupying the half-filled $3d$ shell $L = 0$, therefore:

- one can neglect the single-ion anisotropy, as the crystal field turns out to be ineffective,
- the spin-orbit coupling is relevant only for the virtual excited states $3d^4$ and $3d^6$ (one electron transferred between the $3d$ shell of the dopant and the valence band of the p symmetry), hence the effective p–d exchange coupling does not depend on the orbital degrees of freedom and is given by the isotropic Heisenberg Hamiltonian $H_{pd} = -J_{pd}\,\mathbf{S} \cdot \mathbf{s}$, independently of the symmetry of the term V_{pd} that is responsible for the mixing of the p states (in the valence band) with the d states (on the internal dopant's shell) and necessary for the emergence of the interaction ($J_{pd} \propto |V_{pd}|^2$).

These facts allow to consider the single dopant ion as an $S = 5/2$ spin, localized in the real space, interacting with the external magnetic field (with $g \approx 2$), and with the spins of the carriers (with the exchange coupling J_{pd}).

The complete description of the system consisting of local spins interacting with carriers' spins encounters the following difficulties, typical for the interacting systems, which can not be eliminated by assuming a simplified (one-electron) picture of the carrier subsystem:

1. since $\mathbf{s} = \mathbf{s}(\mathbf{r})$, the interaction is a function of the relative positions of the carrier and the dopant, $\mathbf{r} - \mathbf{R}_i$, and an exact calculation of the matrix element of the interaction requires the knowledge of the carrier's wave function, as well as of the positions of all the dopants and of the function describing the range of the interaction for the relevant combination of the matrix and the dopant;

2. the interaction affects the carrier's wave function; it is no longer a plane wave (the strict translational symmetry is violated);

3. since in contrast to the semiclassical case ($S \to \infty$) the Cartesian components of the tensor operator of the dopant's spin in the Heisenberg Hamiltonian satisfy non-trivial commutation relations, it is not possible to diagonalize the Hamiltonian of the carrier subsystem considering the quantum numbers which describe the state of the local spins as an external field (in relation to the carrier subsytem).

These difficulties can be circumvented through additional approximations. Many of them have a well-established physical grounding and can be formulated in many ways, leading to equivalent results. In particular: neglecting the spatial dependence of the interaction allows to disregard the deviation of the wave functions from the plane waves (and vice versa), resulting in the restoration of the translational symmetry. This approximation is justified if:

1. the interaction is weak, therefore the deviation from the plane wave is small (the relevant dimensionless criterion incolves the exchange constant, the range of the interaction and the mass of the carrier);

2. approximate translational symmetry (homogeneity) of the alloy is preserved;

3. the dopants' concentration is large enough so that they can be considered as a continuum; in that regime the effects of the individual dopants compensate each other rather than sum up, and the deviation of the carrier wavefunction from the plane wave remains small.

If, at the same time, the carrier interacts simultanously with many dopants (this also requires a large enough dopant concentration), it is expected that the quantum effects will disappear (averaging effect). In such case the state of the local spins subsystem is prescribed by the macroscopic magnetization $\mathbf{M}(\mathbf{r})$, and the translational symmetry is violated only by the spatial dependence $\mathbf{M}(\mathbf{r})$. Since $\mathbf{M}(\mathbf{r})$ is a classical field, the p–d exchange interaction term is equivalent to the presence of an external magnetic field (the molecular field), allowing to diagonalize the carrier's Hamiltonian.

The final conclusion of the above discussion is a special case of the mean field approximation. We can therefore expect that, while it is valid for three or more spatial dimensions, and yields correct critical exponents for four and more dimensions, it breaks down in the one- and twodimensional case (the Mermin-Wagner theorem).

The neglection of the quantum effects justified above is equivalent to the limit $S \to \infty$. It is also an inseparable part of the approach based on the Holstein–Primakoff transformation, because it is only in that limit that this transformation is correct, and a prerequisite for application (to the carrier subsystem) of the linear reposponse theory, as the interaction terms comprising the perturbation are not operators in the Hilbert space of the subsystem. It is therefore justified to consider it the common foundation of the different formulations of the present theory of diluted ferromagnetic semiconductors.

Chapter 3

The carrier liquid contribution to magnetization in diluted ferromagnetic semiconductors

A unique feature of the diluted ferromagnetic semiconductors among other ferromagnetic materials is the presence of the two coupled subsystems: the spins of the dopants and of the carriers. As it has been already mentioned in the introduction, in the simplified model it is assumed that the carriers mediate the interaction between the spins, but remain themself insensitive to the external magnetic field. In other words, the carriers' contribution to the macroscopic magnetization is neglected and the latter becomes identical (up to a multiplicative factor proportional to the dopant concentration) with the polarization in the local spins subsystem (and the spin splitting of the band in which the carriers reside). In this approximation one of these quantities (interchangeably) can be regarded as the order parameter describing the ferromagnetic transition.

On the other hand, since the concentration, spin and the gyromagnetic factor of the holes are comparable with the same quantities for the dopants spins, the holes' contribution to the observed magnetization is not negligible. Therefore, if we put apart the methods directly sensitive to the energy levels of the carriers (such as photoemission or optical methods), experimental determination of the dopants concentration requires the subtraction of the holes' contribution from the total measured saturation magnetization.

The hole's contribution to magnetization, $\mathbf{M}_c$, is one of the quantities described by the model which is known as the p–d Zener model and has been calculated (in the spherical approximation for holes) already in the article [4], which introduces that model. This calculation is the starting point of the publication (D1), which aimed at the elimination of the spherical approximation while preserving the general methodology which was based on direct determination of the Landau levels. It was expected that going beyond the spherical approximation would allow to determine the dependence of the holes' magnetization on the direction of the quantization axis for the spin splitting (the direction of the molecular field). Such a dependence, due to the magnetostatic dipole interaction of the subsystems, would contribute to the magnetic anisotropy.

According to the results obtained in (D1),

- the holes' contribution assumes the direction (virtually) parallel to the quantization axis, while the angular dependence of the numerical value of M_c is negligible; this means that the sought contribution to the magnetic anisotropy vanishes;

- the numerical value of M_c is about two times larger than obtained previously in the spherical approximation; this is related to the deviation of the density of states of the valence band in the spherical approximation from the one given by the six-band model (the spherical model reproduces the realistic density of states only at the band's edge) and is important for the sample characterization procedure mentioned above.

In further perspective, the theory of interaction of the holes with external magnetic field is necessary for understanding and quantitative description of the ferromagnetic resonance experiment (FMR). The value of the effective gyromagnetic factor of the coupled subsystems, as observed in this experiment, differs from one known for the free spin of the dopant. From the results obtained for M_c one can tell that, also the simple weighted average of the gyromagnetic factors of the subsystems does not reflect the dependences which were observed in the experiments [5].

To summarize, the results of the publication are important from the point of view of the deficit of macrosopic saturation magnetization and point to the complex character of the dynamics of the coupled subsystems in experiments such as the ferromagnetic resonance.

An intermediate result of the publication is the calculation of the Landau levels in the valence band of GaAs, without the spherical or axial approximations and for arbitrary directions of the magnetic and molecular fields. It required to apply the symbolic computational methods to process the trigonometric expressions present in the hole's Hamiltonian and to diagonalize very large band matrices representing the truncated eigensystem for the Hamiltonian, which in the spherical case is not finite.

As a closing remark let us mention that the holes' magnetization calculated according to the direct method described above is numerically consistent with one obtained within a modern approach, developed recently, which is based on the Berry curvature of the band [6]. This consistency provides strong support for the correctness of both methods and allows to employ them interchangeably, as dictated by the context (the Landau-levels based method allows to take into account the effects such as the orbital diamagnetism, while the advantage of the modern approach is the computational effectiveness).

Chapter 4

The interaction between a photoelectron and the hole bound to a Mn acceptor in GaAs

Because of the different symmetries, the mechanism of the exchange coupling to the local spins is different for the states from the valence band and for the states from the conduction band. The magnitude and sign of the exchange constant reflects that mechanism. It is the potential exchange (the difference in energy between the two-electron state with antiparallel spin directions — and an orbital part symmetric with respect to the interchange of the electrons, and the state with parallel spin directions — and an antisymmetric orbital part of the wavefunction), which is responsible for the s–d exchange coupling. This is why the result of a measurement of the s–d exchange coupling for photoelectrons in GaAs [7, 8], of the opposite sign and much smaller in absolute magnitude with respect to the values typical for magnanese in classical semiconductors, was considered by the authors of these articles as surprising.

Publication (D2) explains the surprising result taking as the starting point the electronic structure of the neutral manganese acceptor in GaAs, known from the measurement of the electron spin resonance [9], i.e. the presence of a hole in the acceptor-bound state. In the explanation which has been proposed in the publication, the photoelectron's spin interacts not only with the spin of the $3d$ electrons of manganese, but also with the spin of the bound hole. In the simplest case this interaction is also described by the Heisenberg Hamiltonian, with the exchange constant following from the form of the hole's wave-function multiplet [10] and of the exchange interaction between the photoelectron and the hole [11].

The calculation of the gyromagnetic factor of the bound hole has made it possible to determine the state of the acceptor-hole complex as a function of the external magnetic field. Since the parameters of the electron–hole exchange interaction are known indirectly from the exchange splitting of the exciton, the electron–hole exchange constant has been expressed in terms of the energies that characterize this splitting. The short-range as well as the long-range component of the interaction have been taken into account. This is important and worth a mention, because their contributions are of similar magnitudes,

while the form of the long-range interaction operator is rather complicated.

The progress in understanding of the investigated system's structure that has been achieved has also allowed to explain the discrepance between the directly measured temperature and the temperature obtained from fitting of the Brillouin function to the observed magnetic field dependence of the spin splitting of photoelectrons, seen in the experiment [7, 8]. In the correct theoretical description the spin splitting is described by a function more complicated than the Brillouin function, and its temperature dependence is rather subtle; therefore the temperature fitted by the authors of [7, 8] does not (directly) reflect the reality.

The presented model has found its application in the description of the electron spin relaxation in GaAs doped with manganese to p-type. The exchange interaction of the electron with the spin of the acceptor leads to the relaxation of the electron's spin, what is known as the Bir-Aronov-Pikus mechanism. In the case of Mn-doped GaAs, the electron interacts with the acceptor-hole complex and one expects that this mechanism is strongly suppressed [12], with the suppression effect significant when the ratio of the exchange constants falls in some numerical range. The values obtained in publication (D2) satisfy this condition, where from we conclude that the model presented therein does apply to the electron-spin relaxation in manganese-doped GaAs.

Chapter 5

Magnetic anisotropy in (Ga,Mn)As layers on GaAs substrates of (113)A orientation

As it has been mentioned in the introduction, the symmetry of the magnetic anisotropy in (Ga,Mn)As is lowered with respect to expectations. In order to understand the origin of the additional component of the anisotropy, we have to find its qualitative features (e.g. the symmetries) and quantify it. As the first step to achieve this, we find the difference between the magnetic anisotropy observed in the experiment and the anisotropy predicted by the model.

The magnetic anisotropy in layers grown on substrates of (001) orientation has three components: the cubic one (resulting from the symmetry of the crystal), (001) uniaxial (resulting from the lattice constant mismatch between the layer and the substrate), and the [110] uniaxial. Hence, the symmetry group is C_{2v} and it is clear which component of magnetic anisotropy requires an extension to the model. As an example of such an extension, one can introduce additional strain.

The anisotropy in layers grown on GaAs substrates of (113)A orientation was the subject of publication (D3). As far as the symmetry is concerned, a layer of (113) orientation has not much in common with a layer on (001)-oriented substrate. The deformation of the layer (resulting from the lattice constant mismatch) is not the same in the two cases and features a shear component in the (113) case; this affects the magnetic anisotropy predicted by the model. If the uncertainty of the sample characteristics is taken into account, it becomes clear that the separation of the additional anisotropy, that we are interested in, from the total observed aniostropy, is ambiguous; therefore, there is some arbitrariness in introducing the additional deformation.

In the theoretical part of publication (D3) it has been assumed that the additional anisotropy has to be referenced to the crystal principal axes, while the additional deformation has only off-diagonal non-vanishing components. The adoption of an appropriate magnitude of the additional deformation allowed to obtain consistency between the model and the experiment. It turned out that while the additional deformation in (001)-oriented

layers has an in-plane component ($\varepsilon'_{xy} \neq 0$), in (113)-oriented layers the additional strain is of an out-of-plane character ($\varepsilon'_{xz} = \varepsilon'_{yz} \neq 0$).

It has been found that the inclusion (in the valence band model) of the terms linear in the momentum and in the off-diagonal components of deformation yields additional contribution to the anisotropy which, although depends in a complicated way on the components of the deformation, is not significant.

The dependence of the free energy on the direction of magnetization has been represented by the coefficients of the expansion into spherical harmonics.

It is important from the point of view of the quantitative consistency between the model and the experiment that the manganese concentration in the samples has been determined from the saturation magnetization taking into account the magnetization of holes, as described in chapter 3.

Chapter 6

The origin of the in-plane magnetic anisotropy in epitaxial layers of (Ga,Mn)As

Achieving an understanding of the origin of the [110] uniaxial anisotropy in (Ga,Mn)As at a quantitative level is important both from of the applicational and the fundamental point of view. This is because the lowered symmetry of the magnetic properties indicates that our previous theory of diluted ferromagnetic semiconductors has been incomplete. In publication (D6) the previous theory has been extended under the presumption that it is the spatial distribution of the dopant itself that is responsible for the lowered symmetry. The building blocks of the extended theory are the description of the surface properties of (Ga,Mn)As and a method to calculate the magnetic anisotropy resulting there from.

The surface property that is essential to achieve the understanding is the difference in energies between the two possible configuration of the Mn dimer on the surface of GaAs. This difference has been calculated by the first author of the publication, employing the DFT code Siesta. The result of the calculation is that a dimer of $[\bar{1}10]$ orientation has lower energy, on the (001) surface of a GaAs crystal, than a dimer of [110] orientation, where from it is expected that the $[\bar{1}10]$-oriented dimers prevail in the bulk (Ga,Mn)As crystal resulting from the growth process.

The method to calculate the resulting magnetic anisotropy is based on the effective strains and the *p–d* Zener model, as follows. The presence of a pair of Mn acceptors in the nearest neighbor position oriented along the preferred direction modifies the properties of the valence band in a way equivalent to a deformation. In the group-theory language, the lowered symmetry allows for the inclusion in the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian of additional terms (invariants), which turn out to posses the same form as the Pikus-Bir Hamiltonian. One can therefore parameterize these additional terms by *effective* strains. In the case of a layer of (001) orientation, the symmetry group (C_{2v}) allows for two effective strains, the shear strain ε_{xy} and the biaxial strain $\varepsilon_{xx} = \varepsilon_{yy} \propto \varepsilon_{zz}$. Finally, the magnetic anisotropy resulting from the effective strains can be calculated in the standard way within the mean field theory (the *p–d* Zener model).

The numerical values of the effective strain parameters can be obtained at the quantitative level in a rather direct way through a DFT calculation with the splitting of the valence band at the Γ point as an intermediate characteristic. This method allows to take into account the effect of lattice relaxation in the dimer's vicinity (the symmetry allows non-vanishing contributions of lattice relaxation to both the effective strains). Alternatively, as described in the publication, the additional term (invariant) can be obtained from perturbation theory within a $\mathbf{k} \cdot \mathbf{p}$ model, surpassing the limits on the supercell that are inherent to present implementations of DFT. In the case of the shear strain component, the numerical values of the two methods differ in magnitudes by a factor of ≈ 2 (in the case of the biaxial strain the variance is greater, and is strongly affected by the size of the supercell).

Proceeding with the perturbation-theory based method requires the knowledge of the potential of a pair of acceptors. The published results were obtained under the assumption of additivity, while the sum of the screened Coulomb part and a Gaussian central cell correction has been adopted as the single-acceptor potential.

According to the above considerations, a systematic analysis requires two parameters for the description of the effects that we are interested in, i.e. an effective biaxial strain has been introduced besides the effective shear strain ε_{xy}. In the presence of an epitaxial strain, the effective biaxial strain is only a small correction. However, in the investigations of samples with different epitaxial strain (both tensile and contractive), the experimental dependence of the perpendicular anisotropy on the difference of lattice constants is a line with a non-zero y-intercept [13, 14], because according to the theory presented in (D6) there is an effective strain even in the absence of any lattice mismatch. We conclude that the extended theory explains also this experimental observation.

Chapter 7

Thermodynamic and thermoelectric properties of (Ga,Mn)As

An alternative model to the *p–d* Zener model of ferromagnetism in (Ga,Mn)As is the impurity band model — or more generally, impurity band models. The alternative models are based on the hypothesis that the impurity-induced states in the band-gap do not merge with the valence band, but rather form a narrow *impurity band*. In the impurity band model the Fermi level and most of the carriers reside in the impurity band, thence the density of states at the Fermi level is enhanced due to small dispersion (large mass) in the impurity band, while the states from the proper valence band are not split by the magnetization. In this situation a comparison of the experimental and theoretical results for the properties which probe the density of states at the Fermi level can provide support for one of the models. Two of such properties, namely the behavior of the specific heat at the critical point and the Seebeck coefficient, have been calculated in publication (D5).

To calculate the critical specific heat one has to extend the mean field theory to include the order parameter fluctuations. In the simplest case a Gaussian distribution of the fluctuations can be assumed. In the Ginzburg-Landau approach the behavior of the system is described in terms of the free-energy functional (the block Hamiltonian):

$$H[\sigma(x)]/k_{\mathrm{B}}T = \int \mathrm{d}^d x \left[a_0 + a_2\,\sigma^2 + a_4\left(\sigma^2\right)^2 + c\,(\nabla\sigma)^2 - h\cdot\sigma\right], \tag{7.1}$$

where $\sigma(x)$ is the configuration of the order parameter, which in the case under consideration is the average of the spins contained in the block near each of the points x, the terms with coefficients a_i constitute an expansion of the free energy dependence on the magnitude of σ, the term with the coefficient c describes the free energy cost of the spatial variation of the order parameter (the spin stiffness), while h is the external magnetic field. Under the present approximations, the terms with the coefficients a_0, a_2, and a_4 are the totals of the contributions from the free spins of the dopants (the integral of the inverse to the Brillouin function) and from the free energy of the carrier Fermi liquid. The contribution from the free energy of the carriers has been obtained numerically, while the stiffness according to the formula from [15], equivalent to the linear response theory

and independently derived employing perturbation theory in [16]. The predictions for the critical specific heat obtained in (D5) employing such a p–d Zener-model based approach do not significantly diverge from the experimentally determined dependences [17].

Another property determined in (D5) is the dependence of the magnetization on the external magnetic field in the critical point of the ferromagnetic transition, $T = T_C$, as predicted by the mean field theory, and namely the coefficient entering the mean-field-theory predicted dependence with the exponent $\delta = 3$. The discrepance by a factor of about 2.5 between the experimental and theoretical values for the investigated sample suggests that only a part of the sample volume is ferromagnetic, e.g. because of the local density of states fluctuations near the metal-insulator transition.

The Seebeck coefficient (the thermopower) has been calculated in the diffusive case (neglecting the phonon and magnon drag), separately for the heavy and the light hole bands for various scattering mechanisms [scattering by acoustic phonons in the GaAs:Be case and ionized impurity scattering in (Ga,Mn)As]. In view of the numerical results, the experimental values of the Seebeck coefficient are consistent with the hypothesis that the carriers in (Ga,Mn)As are holes in the GaAs valence band.

Chapter 8

Hysteresis of magnetoresistance and thermal bistability in magnetic two-dimensional hole gas

The theoretical results published in (D4) were inspired by an experiment performed by the German coauthors. Magnetoresistance in magnetically doped quantum wells was hysteretic as the external magnetic field was swept and exhibited jumps of many order of magnitudes.

The first ingredient of the theory which has been developed in order to explain the observed phenomena is a model for the Mn acceptor in an InAs quantum well. In the presence of a strong exchange coupling between the spins of the dopant and of the bound hole, one expects a bistability of the complex they comprise. The intuition is that the switching of the net magnetic moment of the complex encounters a barrier, which can be surpassed only by simultaneous switching of both spins, i.e. a process involving many bodies. One expects that such processes are rare, as the light hole admixture to the state of the hole in a quantum well implies vanishing of the matrix elements of the x and y components of the hole's spin (j_x, j_y); hence the hole's spin is effectively Ising-like. In such a situtation the dominating mechanism of spin relaxation in the complex has to be the thermal activation over the barrier, whose height is proportional to the hole–dopant exchange constant; thence, the relaxation time is shifted from the milisecond range (the hole's spin relaxation time) to minutes, in the absence of an external magnetic field. This fact seems to be important for possible applications.

The second ingredient of the theory is the termal balance of the system in which there is a strong temperature and magnetic field dependence of resistance, while a weak electron-phonon coupling prevents thermal equilibration of the hole liquid and the lattice. Due to a strong (exponential) temperature dependence of resistance, the system can be found in two states: the low-resistance state (with high power of Joule heating and high temperature) and high-resistance state (low heating and temperature) [18]. The parameters of the resistance model have been fitted to experimental data. The cooling model that has been employed takes into account the coupling of the carriers to acoustic phonons *via* the piezoelectric effect and the deformation-potential term (the Pikus-Bir $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian).

The magnetic field dependence of resistance, as implied by the thermal balance equation, has been parameterized by the hole-liquid temperature, and found to have an S-shape, with evident values of the external magnetic field at which switching between the thermal states occurs.

As already mentioned in the introduction, magnetic hysteresis at a magnetic dopant concentration not sufficient for the emergence of a long range order is an interesting feature of the system under consideration.

Chapter 9

Recapitulation

To recapitulate, the notable results among those contributed by the candidate to the publications in the sequence are:

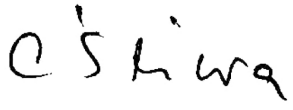
1. a quantitative theory to justify the description of the effect of alloy non-randomness on the properties of band carriers in terms of effective strains and allowing to predict their magnitudes; this result is the basis of the quantitative description of the [110] anisotropy in (Ga,Mn)As;

2. calculation of the Landau levels in semiconductors of zinc-blende structure, in the full six-band $\mathbf{k} \cdot \mathbf{p}$ model of the valence band and in the presence of spin splitting, for arbitrary directions of the external magnetic and molecular fields;

3. a quantitative model of the interaction between the spin of a photoelectron and the complex consisting of a Mn acceptor in GaAs and the bound hole;

4. a model of the magnetic bistability of a similar complex in an InAs quantum well, in the context of the magnetic hysteresis observed experimentally;

5. the calculation of the critical behavior of the specific heat and magnetization as well as of the thermopower in (Ga,Mn)As, which essentially disproves the impurity band hypothesis.



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