The anomalous Hall effect: Recent advances via the geometric-phase approach

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1 Workshop Details

1.1 Details

Timing
Number of days : 0
Start : 2005-07-04
end : 2005-07-06

Location of the activity
CECAM
46 allé e d'Italie
69007 Lyon
France

1.2 Description

We plan to gather in Lyon about 20 senior condensed matter theorists, chosen among those who have contributed significant advances in understanding and computing : electric polarization, orbital magnetisation, anomalous Hall effect, quantum Hall effect, and Berry phases. Notably, we include scientitsts from a wider theoretical-physics community, A few junior participants will be invited later, depending on budget.
The recent developments have occured at a very fast pace in the last two years. This workshop is intended as a very timely forum for discussing some of the unexplored links and consequences. The format and style of a CECAM workshop make the event ideal for discussing open and unsolved problems, work in progress, and other issues normally not reported in a formal talk at a larger (and less specific) conference.

2 Requested Support

CECAM

Psi-k

3 Participant List

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4 Presentation List

Anomalous Hall effect in a two-dimensional electron gas with spin-orbit interaction

Vitalii Dugaev
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Abstract
We discuss the mechanism of anomalous Hall effect related to the contribution of electron states below the Fermi surface (induced by the Berry phase in momentum space). Our main calculations are made within a model of two-dimensional electron gas with spin-orbit interaction of the Rashba type, taking into account the scattering from impurities. We demonstrate that such an "intrinsic" mechanism can dominate but there is a competition with the impurity-scattering mechanism, related to the contribution of states in the vicinity of Fermi surface. We also show that the contribution to the Hall conductivity from electron states close to the Fermi surface has the intrinsic properties as well.

Chern numbers for ferromagnetic metal nanoparticles

Carlo M. Canali
Kalmar University – Sweden, Sweden

Abstract
We argue that ferromagnetic transition metal nanoparticles with fewer than approximately 100 atoms can be described by an effective Hamiltonian with a single giant spin degree of freedom. The total spin S of the effective Hamiltonian is specified by a Berry curvature Chern number that characterizes the topologically non-trivial dependence of a nanoparticle's many-electron wavefunction on magnetization orientation. Interestingly, this simple procedure yields the correct Hund's-3rd-rule values for the ground state degeneracies for isolated (open-shell) atoms. The Berry curvatures and associated Chern numbers have a complex dependence on spin-orbit coupling in the nanoparticle and influence the semiclassical Landau-Liftshitz equations that describe magnetization orientation dynamics. Recent work to evaluate effective giant-spin Hamiltonians for realistic transition metal clusters by performing ab-initio calculations of the Berry curvatures will be discussed.

References

C.M. Canali, A. Cehovin and A.H. MacDonald,
Phys.Rev.Lett. 91, 046805 (2003).

Spin-orbit coupling, complex band structures and ballistic conductance with ultrasoft pseudo-potentials

Andrea Dal Corso
SISSA, Italy

Abstract
The approach proposed by Choi and Ihm∼[1] for calculating the ballistic conductance of open quantum systems has been generalized to deal with magnetic transition metals described by ultrasoft pseudo-potentials.∼[2] I will present some results obtained recently with this method on the spin-resolved conductance of a model Ni nanocontact formed by a three atom monatomic

wire placed between two tips made by seminfinite Ni slabs of (001) orientation.∼[3] Then, I will discuss how this approach can be generalized to treat systems described by spinor wave-functions which allow to describe both non-collinear magnetic structures and systems with spin-orbit coupling.∼[4] As a first result, I will present the complex band structures of a Pt monatomic wire calculated accounting for spin-orbit effects.

References
[1] H.J. Choi and J. Ihm, Phys. Rev. B 59, 2267 (1999).

[2] A. Smogunov, A. Dal Corso, and E. Tosatti, Phys. Rev. B 70, 045417 (2004).

[3] A. Smogunov, A. Dal Corso, and E. Tosatti, in preparation.

[4] A. Dal Corso and A. Mosca Conte, Phys. Rev. B 71, 115106 (2005).

Berry Phase Theory of Charge Effects in Insulators

David Vanderbilt
Rutgers University, United States

Abstract
I will first briefly summarize the Berry-phase theory of electric polarization, which is closely related to the theory of quantized adiabatic charge transport. I will mention some recent topics of interest, including the formulation of a theory of insulators in finite electric field in terms of a coupling of this field to the Berry-phase polarization, and the role of the Berry curvature and metric and the relation of these to each other and to the degree of localization. Returning to the theory of polarization, I will discuss the need for an analogous theory of orbital magnetization, and I will discuss, in general terms, the similarities and differences that may be expected between these two theories.

Kohn localization and the quantum Hall effect

Raffaele Resta
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Abstract
According to Kohn (1964) theory of the insulating state electron localization, defined in an appropriate sense, is the cause for the insulating behavior in any insulator. Since 1999 onwards, the theory of the insulating state has been reformulated in terms of a localization tensor which provides a measure of electron localization. This tensor is an intensive property, geometric in nature, which characterizes the ground wavefunction (not the individual states): it is finite in any insulator and divergent in any metal. In the special case of noninteracting electrons, the localization tensor of the insulating solid is related to the spherical second moment of the Wannier-function charge distribution.
The localization tensor is a ground-state property, related via a fluctuation-dissipation theorem to the system conductivity. So far, the theory has only addressed systems with time-reversal symmetry, in which case the localization tensor is real. I show that in absence of such symmetry

the localization tensor is naturally endowed with an imaginary part, proportional to transverse dc conductivity, and quantized in 2d systems. Therefore electron localization can be regarded as the common cause for both vanishing of the dc conductivity and quantization of the transverse one in QH fluids.

References

W. Kohn, Theory of the insulating state, Phys. Rev. 133, A171 (1964);

R. Resta, Why are insulators insulating and metals conducting?, J. Phys.: Condens. Matter 14, R625 (2002);

R. Resta, Electron localization in the quantum Hall regime, cond-mat/0504054.

Orbital Magnetization in Extended Systems: Numerics and Results

Timo Thonhauser
Rutgers, The State University of New Jersey, United States

Abstract

We present tight-binding calculations of the orbital magnetization in chiral insulators. Our investigations focus on two-dimensional periodic systems with broken time-reversal symmetry and zero Chern number, and on finite samples cut from such systems. Time-reversal symmetry is broken by threading magnetic fluxes through parts of the unit cell in such a way that the net magnetic field remains zero. Results for the calculated magnetization as a function of the flux show that, in the limit of large but finite systems, the orbital magnetization converges to its bulk value as computed in k-space using the formulation presented by Davide Ceresoli. Possible extensions to non-zero Chern numbers and metals will also be discussed.

References

T. Thonhauser, Davide Ceresoli, David Vanderbilt, and R. Resta, submitted to PRL (cond-mat/0505518).

R. Resta, Davide Ceresoli, T. Thonhauser, and David Vanderbilt, ChemPhysChem, in press (2005).

Efficient ab initio calculation of the anomalous Hall conductivity by Wannier interpolation

Ivo Souza
University of California, Berkeley, United States

Abstract

The static intrinsic anomalous Hall conductivity is given by a Brillouin-zone integral of the Berry curvatures of the states below the Fermi surface. It is usually written as a Kubo-formula, which involves a sum over unoccupied states as well. Alternatively, it may be recast in a form where only occupied states appear explicitly. Finally, the non-quantized part can be expressed as a Fermi surface integral[1]. The only ab initio calculations so far[2,3] used the Kubo formula. I will discuss ideas for implementing the other two formulations. The first step is to map the ab initio electronic structure problem onto a tight-binding model, by constructing Wannier functions that accurately describe the ab initio band structure around the Fermi level[4]. The required

quantities can then be evaluated very efficiently at arbitrary k points by Wannier interpolation, without having to perform aditional ab initio calculations. That is particularly advantageous for this problem, since an exceedingly fine sampling of certain regions of the Brillouin zone is needed in order to achieve convergence[3].

References
[1] F. D. M. Haldane, Phys. Rev. Lett. 93, 206602 (2004).

[2] Z. Fang et al,. Science 302, 92 (2003).

[3] Y. Yao et al., Phys. Rev. Lett. 92, 037204 (2004).

[4] I. Souza, N. Marzari, and D. Vanderbilt, Phys. Rev. B 65, 035109 (2002).

Orbital Magnetization in Extended Systems: Theory
Davide Ceresoli
SISSA, Italy
Abstract
The magnetic dipole moment of any finite sample is well defined, while it becomes ill defined in the thermodynamic limit, due to the unboundedness of the position operator. The corresponding electrical problem, where surface charges and bulk polarization appear as entangled, has been solved about one decade ago by the modern theory of polarization, based on a Berry phase. We follow a similar path here, providing a bulk expression for orbital magnetization for any lattice-periodical, though time-reversal breaking, Hamiltonian. We therefore limit ourselves to cases where the macroscopic (i.e. cell-averaged) magnetic field vanishes. For crystalline insulators we express the bulk magnetization in terms of Wannier functions, and we then transform the expression into a Brillouin-zone integral involving the occupied Bloch orbitals. Interestingly, the final expression remains well-defined even for metals, but it is not yet clear whether it is correct in that case.

The Quantum Spin Hall Effect
Charles Kane
University of Pennsylvania, United States
Abstract
We show that the intrinsic spin orbit interaction in a single plane of graphene converts the ideal two dimensional semi metallic groundstate of graphene into a quantum spin Hall (QSH) state [1]. This novel electronic phase shares many similarities with the quantum Hall effect. It has a bulk excitation gap, but supports the transport of spin and charge in gapless ”spin filtered” edge states on the sample boundary. We show that the QSH phase is associated with a Z_2 topological invariant, which distinguishes it from an ordinary insulator [2]. The Z_2 classification, which is defined for any time reversal invariant Hamiltonian with a bulk excitation gap, is analogous to the Chern number classification of the quantum Hall effect. We argue that the QSH phase is topologically stable with respect to weak interactions and disorder. The QSH phase exhibits a finite (though not quantized) dissipationless spin Hall conductance even

in the presence of weak disorder, providing a new direction for realizing dissipationless spin transport.

References

1. C.L. Kane and E.J. Mele, cond-mat/0411737
2. C.L. Kane and E.J. Mele, cond-mat/0506581

Spin Hall Effect and Spin Hall Spin Accumulation

Allan H. MacDonald
University of Texas at Austin, United States

Abstract

The controlled generation of localized spin-densities is a key enabler of semiconductor spintronics. Finite spin-densities in semiconductors have traditionally been generated by external magnetic fields, by circularly polarized light sources, or by spin injection from ferromagnetic metals. Recently there has been considerable interest in an alternate strategy in which edge spin densities are generated electrically via the spin Hall effect, em i.e. (in a planar device) by the current of spins ($j^ z_H$) oriented perpendicular to the plane that is generated by and flows perpendicular to an electric field. Practical interest in this effect is motivated by arguments that, at least in principle, it may enable low power consumption electronic devices.
The spin Hall effect has traditionally been thought of as a consequence of skew-scattering citeDyakonov:1971_b,Hirsch:1999_a,Kato:2004_d, spin-dependent chirality in impurity scattering that ocurs in systems with spin-orbit coupling. Recently it has been recognized that the spin Hall effect also has an intrinsic contribution due to spin-orbit coupling in a perfect crystal. I will discuss the various contributions to the spin Hall conductivity and their relationship to the strongly analogous contributions the Hall conductivity of a ferromagnet. One broad classification of contributions is that the spin Hall conductivity is the sum of an interband coherence response contribution that is often dominated by an intrinsic part and a skew scattering contribution.
In isotropic two-dimensional electron systems spin-orbit interactions can normally be modelled as momentum dependent Zeeman fields which always point in the plane. In these systems the skew scattering contribution is absent. For a two-dimensional hole gas with strong spin-orbit interactions the spin Hall conductivty is well approximated by its intrinsic contribution.
The main observable consequence of the spin Hall effect is the spin accumulations near sample edges to which they give rise. Because spin is not conserved in systems with spin-orbit interactions, there is no unique definition of the spin current. The measure of merit of a particular spin-current definition is its utility for the evaluation of the edge spin accumulations associated with the spin Hall effect. There is not, as yet, a useful and general theory of these spin accumulations in systems with strong spin-orbit interactions. I will present and discuss numerical results which indicate that for a two-dimensional hole gas the edge spin-density is proportional to the spin Hall current and inversely proportional to the hole gas Fermi velocity, and that it is localized within a spin-precession length of the edge.

Disorder effects in Berry phase phenomena

Naoto Nagaosa

Department of Applied Physics, The University of Tokyo, Japan

Abstract
Disorder effects such as the impurity scattering play crucial roles in the transport phenomena and dielectric phenomena governed by the Berry phase curvature. Especially the debates on the intrinsic and extrinsic mechanism of anomalous Hall effect and spin Hall effect still continue with lots of confusions. I will talk on the recent advances on these problems. We found that the magnetic monopole and the associated non-perturbative aspect is essential for the intrinsic mechanism. I will also discuss the role of Anderson localization in anomalous Hall effect and charge pumping.

Pseudopotential Hamiltonian in Magnetic field: the orbital magnetism within a pseudopotential framework

Francesco Mauri
Universite Pierre et Marie Curie, France

Anomalous Hall Effect in Ferromagnets

Patrick BRUNO
Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

Berry Phase Theory of the Anomalous Hall Effect

F. Duncan M. Haldane
Princeton University, United States

Abstract
The Karplus-Luttinger formula for the intrisic AHE has been recognized as an integral over the "Berry Curvature" of all occupied Bloch states. This formula resembles the Landau diamagnetism formula, and appears not to be a Fermi surface formula, in violation of the fundamental principle that all transport processes occur at the Fermi level. Recently I have shown that it is in fact the sum of a quantized part associated with topologically-non-trivial occupied bands, and non-quantized part determined entirely at the (bulk) Fermi surface. There is a simple geometrical formula for the Fermi surface part that is valid in interacting Fermi liquids (like the Luttinger Fermi surface volume theorem, to which it is related); the quantized part is also a Fermi level effect associated with chiral edge states at the Fermi level, which are necessaily present if there are fully-occupied bands with non-trivial topology. These results prompt a new look at ingredients of Fermi liquid theory that were not recognized when that theory was developed. A subtlety about the "Berry curvature" of Bloch states will also be discussed: it encodes the embedding of Hilbert space in real space in addition to properties of the Bloch wavefunctions.

References

F. D. M. Haldane, Phys. Rev Lett. 93, 206602 (2004)

Berry phase correction to electron density of states in solids

Qian Niu

University of Texas at Austin, United States

Abstract
Liouville's theorem on the conservation of phase space volume is violated by Berry phase in the semiclassical dynamics of Bloch electrons. This leads to a modification of the phase space density of states, whose significance is discussed in a number of examples: field modification of the Fermi-sea volume, connection to the anomalous Hall effect, and a general formula for orbital magnetization. The effective quantum mechanics of Bloch electrons is also sketched, where the modified density of states plays an essential role.

On A Proper Definition of Spin Current

Qian Niu
University of Texas at Austin, United States

Abstract
The conventional definition of spin current is incomplete and unphysical in describing spin transport in systems with spin-orbit coupling. A proper and measurable spin current is established in this study, which fits well into the standard framework of near-equilibrium transport theory and has the desirable property to vanish in insulators with localized orbitals. Our theory predicts opposite signs of spin Hall coefficients for a few semiconductor models, urging critical tests of the concept by experiments and numerics.

Ab initio calculation of spin Hall effect in semiconductors and anomalous Hall effect in ferromagnetic insulators

Guang-Yu Guo
National Taiwan University, Department of Physics, Taipei 106, Taiwan, Republic of China

Abstract
Spin current generation is an important issue in the emerging spintronics technology. Recent proposals of the intrinsic spin Hall effect by Murakami et al [1] and Sinova et al [2], are therefore fascinating. This spin Hall effect would enable spin current generation in semiconductors without magnetic field or magnetic materials, and promise a tremendous potential of combining spintronics with the well-developed semiconductor technology. However, the recent proposals of the intrinsic spin Hall effect have been subject to careful scrutinies. In particular, Wang and Zhang [3] argued that spin symmetry consideration would rule out the possibility of such a spin current in the semiconductors described by the Luttinger Hamiltonian which was used in [1]. On the other hand, Zhang and Yang [4] point out that the intrinsic spin Hall effect predicted in [2], in a two-dimensional electron gas in semicoductors, would be exactly cancelled by the intrinsic orbital-angular-momentum Hall (orbital) effect. Therefore, fundamental questions such as the existence of the intrinsice spin Hall effect in semiconductors structures and that whether it would be cancelled out by the orbital Hall effect, remain unsolved despite enormous recent efforts. In this talk, we report our ab initio relativistic band theoretical calculations on the intrinsic spin Hall effect in the archetypical semiconductors Si, Ge, GaAs and AlAs [5]. Our results cover a large range of hole concentration which is beyond the validity regime of the Luttinger model. We find that intrinsic spin Hall conductivity in hole-doped semiconductors Ge, GaAl

and AlAs is large, showing the possibility of spin Hall effect beyond the Luttinger Hamiltonian. The calculated orbital Hall conductivity is one order of magnitude smaller, indicating no cancellation between the spin and orbital Hall effects in bulk semiconductors. Furthermore, it is found that the spin Hall effect can be strongly manipulated by strains, and that the ac spin Hall conductivity in the semiconductors is large in pure and as well as doped semiconductors.

References

[1] S. Murakami, N. Nagaosa, and S.-C. Zhang, Science 301, 1348 (2003).
[2]ÅJ. Sinova et al., Phys. Rev. Lett. 92, 126603 (2004).
[3] X. Wang, and X.-G. Zhang, J. Magn. Magn. Mater. 288, 297 (2005).
[4] S. Zhang, and Z. Yang, Phys. Rev. Lett. 94, 66602 (2005).
[5] G.Y. Guo, Y. Yao, and Q. Niu, Phys. Rev. Lett. 94, 226601 (2005).

Spin Hall Effect

Tomas Jungwirth
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Spin Hall Effect

Jairo Sinova
Texas A&M University, United States

The anomalous Hall effect in re-entrant AuF alloys and the real space Berry phase

Ian Campbell
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Abstract

The Hall effect has been studied in a series of AuFe samples in the re-entrant concentration range, as well as in the spin glass range. The data demonstrate that the degree of canting of the local spins strongly modifies the anomalous Hall effect, in agreement with model predictions associating canting, chirality and the ”real space Berry phase”. The canonical parametrization of the Hall signal for magnetic conductors becomes inappropriate when local spins are canted.

5 Program

Day 1: July 04 2005

Session : 1 Anomalous Hall effect
09:00 to 09:30 : Welcome

09:30 to 10:30 : Presentation
Anomalous Hall Effect in Ferromagnets
Patrick BRUNO

10:30 to 11:00 : Coffee Break

11:00 to 12:00 : Presentation
Berry Phase Theory of the Anomalous Hall Effect
F. Duncan M. Haldane

Session : 2 Orbital magnetization
14:00 to 15:00 : Presentation
Berry Phase Theory of Charge Effects in Insulators
David Vanderbilt

15:00 to 15:15 : Presentation
Orbital Magnetization in Extended Systems: Theory
Davide Ceresoli

15:15 to 15:30 : Presentation
Orbital Magnetization in Extended Systems: Numerics and Results
Timo Thonhauser

15:30 to 16:00 : Coffee Break

16:30 to 16:50 : Presentation
Pseudopotential Hamiltonian in Magnetic field: the orbital magnetism within a pseudopotential framework
Francesco Mauri

16:50 to 18:00 : Discussion

16:00 to 16:30 : Presentation
Berry phase correction to electron density of states in solids
Qian Niu

Day 2: July 05 2005

Session : 3 Spin Hall effect
09:00 to 10:00 : Presentation
Spin Hall Effect and Spin Hall Spin Accumulation
Allan H. MacDonald

10:00 to 10:30 : Presentation
The Quantum Spin Hall Effect
Charles Kane

10:30 to 11:00 : Coffee Break

11:00 to 11:30 : Presentation
Ab initio calculation of spin Hall effect in semiconductors and anomalous Hall effect in ferromagnetic insulators
Guang-Yu Guo

11:30 to 11:45 : Presentation
Spin Hall Effect
Tomas Jungwirth

11:45 to 12:00 : Presentation
Spin Hall Effect
Jairo Sinova

Session : 4 Spin currents; localization
14:00 to 14:30 : Presentation
On A Proper Definition of Spin Current
Qian Niu

14:30 to 15:00 : Discussion

15:00 to 15:30 : Coffee Break

15:30 to 16:00 : Presentation
Kohn localization and the quantum Hall effect
Raffaele Resta

16:00 to 16:30 : Presentation
Efficient ab initio calculation of the anomalous Hall conductivity by Wannier interpolation
Ivo Souza

16:30 to 17:00 : Presentation
Chern numbers for ferromagnetic metal nanoparticles
Carlo M. Canali

Day 3: July 06 2005

Session : 5 Disorder; spin-orbit
09:00 to 10:00 : Presentation
Disorder effects in Berry phase phenomena
Naoto Nagaosa

10:00 to 10:30 : Presentation
The anomalous Hall effect in re-entrant AuF alloys and the real space Berry phase
Ian Campbell

10:30 to 11:00 : Coffee Break

11:00 to 11:30 : Presentation
Spin-orbit coupling, complex band structures and ballistic conductance with ultrasoft pseudo-potentials
Andrea Dal Corso

11:30 to 12:00 : Presentation
Anomalous Hall effect in a two-dimensional electron gas with spin-orbit interaction
Vitalii Dugaev

6 Organizer's report

6.1 Conclusions.

There have been sweeping advances since 2002 in understanding and computing the anomalous Hall effect (AHE) from first principles. The Hall resistivity of ferromagnets has an ordinary contribution (proportional to the external magnetic field strength), and an anomalous contribution (often assumed proportional to the sample magnetization). The phenomenon of AHE was discovered by E.R. Hall in 1881, shortly after his discovery of the normal effect. Nonetheless its interpretation has been controversial until recently. It is by now clear that the AHE is dominated by band-structure effects and can be computed as a suitable Berry phase. Other closely related, and equally controversial issues, concern the spin Hall effect, and orbital magnetization in extended systems. All of these issues have possible relevant implications for spintronics applications.
The above topics have been thoroughly and lively discussed in the workshop. Besides the "formal" presentations, an important part of the meeting has been in the long discussions, augmented with a few informal short presentations. We have gathered in Lyon 21 condensed matter theorists (plus a senior experimentalist), chosen among those who have in the past contributed significant advances in understanding and computing: electric polarization, orbital magnetization, anomalous Hall effect, quantum Hall effect, and Berry phases. Notably, we included scientists from the computational electronic-structure community, as well as scientists from a wider theoretical-physics community. It is remarkable that, while the preliminary participants' list was built on the basis of a generic cultural interest, some people in this list started working more specifically on the workshop topics only AFTER the workshop was proposed and approved.
Given the nature of the event, most participants were senior ones, where some junior collaborators of the senior participants attended as well. Two young US participants profited of the NSF support under the CECAM-NSF agreement.
Some participants, including the most seniors of them, sent a feedback of real enthusiasm. It is remarkable that–despite the partial support available under the CECAM rules–almost one half of the participants travelled from overseas (USA, Japan, Taiwan) expressly for this very short event.
The success of the workshop owes to two main features. (1) Timeliness, demonstrated by the fact that a large number of important papers (e.g. PRLs), and preprints posted on the web, have appeared AFTER the workshop was proposed and approved. (2) By means of participants' selection, care was taken to foster the interaction between physicists belonging to different communities: quantum-Hall (mostly analytical approach) and electronic structure (mostly computational approach).

6.2 Recommendations.

My own recommendations for any CECAM workshop (DO and DO NOT):
DO: Choose a hot topic, possibly which underwent recent sweeping progress.

DO NOT: Choose the participants from within a small pool, which meets already (even without CECAM) several times per year. Instead, try to blend the participants from communities as diverse as possible.