CECAM WORKSHOP: Orbital Magnetization in Condensed Matter
Dates : Jun 15, 2009 - Jun 17, 2009
Location : CECAM-HQ-EPFL, Lausanne, Switzerland

SUMMARY

Macroscopic magnetization is a fundamental concept that all undergraduates learn about in elementary courses. In view of this, it is truly extraordinary that before 2005 there was no generally accepted formula for the macroscopic orbital magnetization in condensed matter. This workshop has been intended a very timely forum for discussing the many open issues.

DESCRIPTION

Orbital magnetization--as opposed to spin magnetization--occurs whenever time-reversal symmetry is broken in the spatial wavefunction. For instance, in a ferromagnet the spin-orbit interaction transmits the symmetry breaking from the spin degrees of freedom to the spatial (orbital) ones; the two contributions to the total magnetization can be resolved experimentally. Other examples include the induced magnetization in applied magnetic fields, or in any other time-reversal-symmetry breaking perturbations. Whenever the unperturbed system is nonmagnetic, the induced magnetization is 100% of the orbital kind.

Sweeping advances are occurring at the time of the workshop in the field of orbital magnetization, and a "modern theory" is in development. The key formulas are resemblant of (but more complex than) the Berry-phase formulas of the modern theory of electric polarization, developed in the 1990s, and by now famous. Formulas for orbital magnetization discussed at the workshop are: (1) for crystalline solids, either metallic or insulating, at the mean field level (HF or Kohn-Sham); (2) for noncrystalline insulators at a the mean-field level (such as for Car-Parrinello simulations). Some progress has been achieved even in the case of a correlated wavefunction, but the ultimate theory has not yet been developed.

Mostly model Hamiltonians have been addressed before 2009; the first results from a first-principle implementation were just submitted in preprint form, and discussed at the workshop ([5] by Ceresoli et al.). Concerning applications of the novel theory, a promising novel scheme for evaluating NMR shielding tensors has been proposed ([8] by Thonhauser et al.); its first-principle implementation was also just submitted in preprint form at the workshop time.

Another open issue relates orbital magnetization (which is a ground state property) to magnetic circular dichroism, by means of magneto-optical sum rules widely used by X-ray spectroscopists at synchrotron facilities. This was discussed by the leading specialists, also in relationship to Ref. [6] below.

Key references:
[1] D. Xiao, J. Shi, and Q. Niu, Phys. Rev. Lett. 95, 137204 (2005).
[2] T. Thonhauser, D. Ceresoli, D. Vanderbilt, and R. Resta, Phys. Rev. Lett. 95, 137205 (2005).
[3] D. Ceresoli, T. Thonhauser, D. Vanderbilt, and R. Resta, Phys. Rev. B 74, 024408 (2006).
[4] J. Shi, G. Vignale, D. Xiao, and Q. Niu, Phys. Rev. Lett. 99, 197202 (2007).
[5] D. Ceresoli, U. Gerstmann, A.P. Seitsonen, and F. Mauri, http://arxiv.org/abs/0904.1988.
[6] I. Souza and D. Vanderbilt, Phys. Rev. B 77, 054438 (2008).
[7] D. Xiao, J. Shi, D.P. Clougherty and Qian Niu, Phys. Rev. Lett. 102, 087602 (2009)
[8] T. Thonhauser, A.A. Mostofi, N. Marzari, R. Resta, D. Vanderbilt,
http://arxiv.org/abs/cond-mat/0709.4429.
[9] D. Ceresoli and R. Resta, Phys. Rev. B 76, 012405 (2007).

ASSESSMENT AND IMPACT

All of the key players in this very novel field were present at the workshop. Some of them presented unpublished results and work in progress, besides part of the very successful published work. Most researchers went back home with novel ideas to explore and projects to develop (together with they collaborators) in the forthcoming months.

PARTICIPANT LIST

Organizers

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FINAL PROGRAMME OF THE MEETING

Day 1 - June, 15th 2009
Fundamentals
09:20 to 09:30 - Welcome
09:30 to 10:00 - Raffaele Resta
Macroscopic magnetization: Analogies to and differences from the case of
electrical polarization
10:00 to 10:15 - Discussion
10:15 to 10:45 - David Vanderbilt

Theory of orbital magnetization in crystalline systems
10:45 to 11:00 - Discussion
11:00 to 11:30 - Coffee Break
11:30 to 12:00 - Qian Niu
Theory of Orbital Magnetization and its Generalization to Interacting Systems
12:00 to 12:15 - Discussion
12:15 to 14:00 - Lunch Break
Experiment
14:00 to 14:30 - Patrick Bruno
Hall Effect, Generalized Einstein Relation, and Berry Phase
14:30 to 14:45 - Discussion
14:45 to 15:15 - Gerrit van der Laan
Sum rules for E1-E1 x-ray absorption
15:15 to 15:30 - Discussion
15:30 to 15:55 - Andrei Rogalev
X-ray Magnetic Circular Dichroism Studies of Paramagnetics
15:55 to 16:00 - Discussion
16:00 to 16:15 - Coffee Break
16:15 to 16:45 - Fabrice Wilhelm
Induced orbital magnetism of 5d transition metals studied with XMCD
16:45 to 17:00 - Discussion
Calculations
17:00 to 17:20 - Davide Ceresoli
First principles theory of the orbital magnetization: ferromagnetic metals and organometallic complexes
17:20 to 17:30 - Discussion
17:30 to 17:45 - Yugui Yao
First principles calculations of Orbital magnetization-Preliminary Results
17:45 to 17:50 - Discussion

Day 2 - June, 16th 2009
Molecules and ions
09:00 to 09:30 - E.K.U. Gross
Exact Born-Oppenheimer decomposition of the complete electron-nuclear wave function
09:30 to 09:45 - Discussion
09:45 to 10:15 - Paolo Lazzeretti
Induced orbital paramagnetism in BH, CH+, C4H4, and C8H8 systems
10:15 to 10:30 - Discussion
10:30 to 10:50 - Uwe Gerstmann
Ab initio calculation of the electronic g-tensor beyond perturbation theory: diatomic molecules and defects in semiconductors
10:50 to 11:00 - Discussion
11:00 to 11:15 - Coffee Break
11:15 to 11:40 - Philippe Sainctavit
Is there a relation between the magnetic anisotropy of a single molecule magnet and the orbital magnetic moments of its ions ?
11:40 to 11:45 - Discussion
11:45 to 12:15 - Guang-Yu Guo
Orbital magnetization, XMCD and magnetic hyperfine field
12:15 to 12:30 - Discussion
12:30 to 14:00 - Lunch Break
Theory developments (1)
14:00 to 14:30 - Ivo Souza
What is the most physical way of dividing up the orbital magnetization into two gauge-invariant parts?
14:30 to 14:45 - Discussion
14:45 to 15:05 - Raffaele Resta
Single k-point formulas for the electrical and magnetic cases
15:05 to 15:15 - Discussion
15:15 to 15:45 - Sergej Savrasov
Calculations of Magnetic Exchange Interactions in d- and f- Electron Systems
15:45 to 16:00 - Discussion
16:00 to 16:15 - Coffee Break
Topological insulators

16:15 to 16:45 - David Vanderbilt
Orbital magnetoelectric effects and topological insulators
16:45 to 17:00 - Discussion
17:00 to 17:20 - Ming-Che Chang
Optical properties of topological insulator
17:20 to 17:30 - Discussion
19:30 to 21:30 - Dinner

Day 3 - June, 17th 2009
Theory developments (2)
09:00 to 09:30 - Jonathan Yates
Spin-spin coupling in the solid state
09:30 to 09:45 - Discussion
09:45 to 11:05 - Anne-Christine Uldry
Spin and orbital moments in the Fe-Cr alloy
10:05 to 10:15 - Discussion
10:15 to 10:45 - Timo Thonhauser
Orbital Magnetization and its Connection to NMR Chemical Shifts
10:45 to 11:00 - Discussion
11:00 to 11:30 - Coffee Break
12:00 to 12:15 - Discussion
11:30 to 12:00 - Junren Shi
Polarization Induced by Inhomogeneity
12:00 to 12:15 - Discussion
12:15 to 14:00 - Lunch Break
14:00 to 16:00 - Discussion