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Skyrmions and topological defects

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Abstract. The lecture will start by introducing the topological theory of defects in condensed matter. The first work in this direction concerned magnetism, and the general theory has been developed by Maurice Kléman and coworkers [1,2], with an important application to liquid crystals. A second generalization, sketched by Louis Michel and developed by Hans-Rainer Trebin [3], applied topology to define topologically stable structures, also called topological solitons. Skyrmions are one instance of these [4]. Two ways of experimentally "measuring topology" via physical quantities will be then introduced, namely the gyrotropic deflection of moving topological solitons [5], and the topological Hall effect. The dynamics of topological solitons will be shown to reveal that topology alone does not describe all the physics, as for example the chirality of the textures can play a big role. Furthermore, ways to "weigh topology" will be described, through the estimation of the energetic cost to violate it (skyrmions creation and annihilation). The lecture will be based on experiments using skyrmions, both recent and older.

Suggested introductory readings

1. G. Toulouse, M. Kléman, Principles of a classification of defects in ordered media, J. Physique Lett. **37**, L149-151 (1976).
2. N.D. Mermin, The topological theory of defects in ordered media, Rev. Mod. Phys. **51**, 591-648 (1979); M. Kléman, *Points, lines and walls* (Wiley, New York, 1983).
3. L. Michel, Symmetry defects and broken symmetry. Configurations hidden symmetry, Rev. Mod. Phys. **52**, 617-651 (1980); H.-R. Trebin, The topology of non-uniform media in condensed matter physics, Adv. Phys. **31**, 195-254 (1982).
4. T.H.R. Skyrme, A non-linear theory of strong interactions, Proc. Roy. Soc. A **247**, 260-278 (1958); A unified field theory of mesons and baryons, Nucl. Phys. **31**, 556-569 (1962).
5. A.A. Thiele, Steady-state motion of magnetic domains, Phys. Rev. Lett. **30**, 230-233 (1973); Application of the gyrocoupling vector and dissipation dyadic in the dynamics of magnetic domains, J. Appl. Phys. **45**, 377-393 (1974).

Skyrmions et défauts topologiques

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Résumé. Ce cours commencera par une présentation de la théorie topologique des défauts en matière condensée. Les premiers travaux en ce sens se situent dans le domaine du magnétisme, la théorie générale ayant été ultérieurement développée par Maurice Kléman et collaborateurs [1,2], avec une application importante aux cristaux liquides. Une seconde généralisation, esquissée par Louis Michel et développée par Hans-Reiner Trebin [3], utilise la topologie pour définir les structures stables topologiquement, appelées aussi solitons topologiques. Les skyrmions sont un cas particulier de telles structures [4]. On introduira ensuite deux manières de « mesurer expérimentalement la topologie », via des quantités physiques qui font intervenir le nombre topologique associé, à savoir la déflexion gyrotropique dans la dynamique de solitons topologiques [5], ainsi que l'effet Hall topologique. En étudiant la dynamique des solitons topologiques, on montrera que la classification topologique n'épuise pas la physique, car elle laisse de côté la chiralité qui joue aussi un grand rôle. On passera enfin aux manières de « peser la topologie », via l'estimation du coût énergétique à violer la topologie (création, annihilation de skyrmions). Le cours s'appuiera en partie sur des expériences récentes sur les skyrmions, ainsi que sur d'autres expériences plus anciennes.

Suggestions de lecture

6. G. Toulouse, M. Kléman, Principles of a classification of defects in ordered media, J. Physique Lett. **37**, L149-151 (1976).
7. N.D. Mermin, The topological theory of defects in ordered media, Rev. Mod. Phys. **51**, 591-648 (1979); M. Kléman, *Points. Lignes. Parois* (Éditions de Physique, Orsay, 1977).
8. L. Michel, Symmetry defects and broken symmetry. Configurations hidden symmetry, Rev. Mod. Phys. **52**, 617-651 (1980); H.-R. Trebin, The topology of non-uniform media in condensed matter physics, Adv. Phys. **31**, 195-254 (1982).
9. T.H.R. Skyrme, A non-linear theory of strong interactions, Proc. Roy. Soc. A **247**, 260-278 (1958); A unified field theory of mesons and baryons, Nucl. Phys. **31**, 556-569 (1962).
10. A.A. Thiele, Steady-state motion of magnetic domains, Phys. Rev. Lett. **30**, 230-233 (1973); Application of the gyrocoupling vector and dissipation dyadic in the dynamics of magnetic domains, J. Appl. Phys. **45**, 377-393 (1974).

Lecture on condensed matter magnetism

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Abstract. The aim of this lecture is to recall the basis of magnetism. The lecture will start with the isolated atom and the definition of the atomic magnetic moment. The Hund's rules, spin-orbit coupling and crystal field theory will be presented. Then the thermodynamics of an assembly of such isolated magnetic moments will be considered. The different types of interactions between magnetic moments will be described as well as the resulting collective behaviors (static and dynamics). From this microscopic description, the macroscopic behavior of magnetic materials adapted to micromagnetic studies will be succinctly described. Finally an emphasis will be given to the tools devoted to the study of magnetic materials and to the modern trends of research in this field of magnetism.

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Growth of epitaxial heterostructures

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Abstract. Recent advances in solid state sciences include for example the discovery of new, topologic, electronic phases of matter or the evidence of emergent phenomena at interfaces between two materials having distinct electronic and/or magnetic properties. In such a context, thin film growth plays a crucial role: the ability to grow state of the art heterostructures paves the way towards the study of new phenomena and properties. In this lecture, the fundamental concepts of thin film growth will be introduced. The kinetic and thermodynamic aspects of nucleation and growth of heterostructures [1, 2] will be discussed and the different growth modes will be detailed. A particular emphasis will be put on epitaxial structures that enable strain engineering of the physical properties. The basic principles of molecular beam epitaxy (MBE) and pulsed laser deposition (PLD) will be exposed. Methods to monitor the growth in situ in real time and ex situ will also be discussed. Recent examples taken from the literature, in which the growth of state-of-the-art epitaxial heterostructures (either by MBE or PLD) is crucial, will illustrate the points introduced during this lecture

References

[1] J. A. Venables, *Introduction to Surface and Thin Film Processes* (Cambridge University Press, Cambridge, 2000)

[2] H. Lüth, *Solid Surfaces, Interfaces and Thin Films* (Springer-Verlag, Berlin Heidelberg, 2001)

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Ultrafast pump-probe experiments: application to correlated electron systems

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Abstract. Among strongly correlated electron systems, superconductors and materials exhibiting metal-insulator transitions are usually characterized by strong electron-electron and electron-phonon couplings. Studying their electronic structure, atomic structure and phonon spectrum provides insight on the mechanisms of their phase transitions, which take place on quasi-adiabatic pathways. Correlated electrons systems also display fascinating out-of-equilibrium physics, in the form of ultra-fast symmetry changes known as photoinduced phase transitions, and occurrence of new, transient states. Out-of-equilibrium states are typically obtained by irradiation with ultra-short optical laser pulses. Those induce electronic transitions on a timescale for which the lattice is considered to be frozen, leading to a transient decoupling between electronic and lattice degrees of freedom. One then has the opportunity to study their mutual interaction during the relaxation process and, in certain cases, to modify their interaction in a controlled way. Ultrafast photo-induced dynamics of atomic and electronic structures are studied directly in the time domain, during so-called "pump-probe" experiments. The sample is excited (pumped) by a fs optical laser pulse, and probed after a delay Δt by a light pulse in the infrared, visible, UV or X-ray range of wavelengths. In the last decades, various experiemental techniques were adapted to the pump-probe scheme, among which ARPES and X-ray diffraction that are especially relevant for studying correlated electron systems. The lecture will present various pump-probe setups used nowadays and exemples of current research topics involving out-of equilibrium dynamics.

Suggested introductory readings (textbook, review or articles)

1. P. Beaud, A. Caviezel, …, S.L. Johnson, U. Staub, Nature Materials **13**, 923 (2014)
2. S. Hellmann, T. Rohwer, …, M. Bauer, K. Rossnagel, Nature Comm. **3**, 1069 (2012)
3. L. Guérin, J. Hébert, …, H. Cailleau, E. Collet, Phys. Rev. Lett. **105**, 246101 (2010) // C. Laulhé, T. Huber, …, S.L. Johnson, S. Ravy, Phys. Rev. Lett. **118**, 247401 (2017)
4. R. Mankowsky, M. Först, A. Cavalleri, Rep. Prog. Phys. **79**, 064503 (2016)

(High field) Transport properties of strongly correlated metals

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Abstract. Transport properties is often the first things to be measured but the last to be understood. Here, I will describe how the transport properties can be a powerful probe of strongly correlated metals. After a brief introduction on the different transport coefficients and on the experimental techniques, the behaviour of the low temperature resistivity of correlated metals will be discussed, in particular the hallmarks of Fermi liquid behaviour and quantum critical point. Another part will be devoted to measurements in high magnetic fields. For instance, it allows for probing quantum oscillations that yield a measure of the Fermi surface area in momentum space. The use of magnetic fields to reveal the underlying ground state of high T_c superconductor will be summarized.

Suggested introductory readings (textbook, review or articles)

1. A.A. Abrikosov, *Fundamentals of the theory of metals* (North Holland, 1988)
2. D. Shoenberg, *Magnetic Oscillations in Metals* (Cambridge Univ. Press, 1984)
3. N. Hussey, J. Phys.: Condens. Matter **20** 123201 (2008)
4. S.E. Sebastian and C. Proust. *Annual Review of Condens. Matter Physics* **6**, 411 (2015)

Quantum Magnetism of Effective Models

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Abstract. In this lecture, I will review the properties of the quantum Heisenberg model and of some of its extensions, including an external magnetic field, with emphasis on the physical properties of the various types of phases that have been proposed and sometimes observed: magnetic long-range order, spin nematic order, algebraic order, gapped systems, Resonating Valence Bond liquids, and chiral spin liquids. In all cases, I will discuss simple models where the relevant physics has been demonstrated, and whenever possible I will mention experimental realizations. On the way, I will also discuss the main theoretical and numerical tools that have proven most useful to describe this very rich family of quantum states of matter.

Suggested introductory readings (textbook, review or articles)

1. Introduction to Frustrated Magnetism, C. Lacroix, P. Mendels, F. Mila (Eds.), Springer (2011).
2. Frustrated Spin Systems, F. Mila, Lecture Notes of the Autum School on Correlated Electrons 2015, Eva Pavarini, Erik Koch, and Piers Coleman (Eds.), Forschungszentrum Jülich GmbH, Chapter 7.

ARPES and experimental electronic structure of correlated materials

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Abstract. Angle-resolved photoemission spectroscopy (ARPES) is a powerful technique to study the microscopic properties of solids. ARPES gives direct access to the band structure of a material, and provides valuable information about the many-body interactions affecting such band structure. This lecture will introduce the basic aspects of ARPES, from a synopsis of currently used instrumentation to its application in the study of correlated-electron systems. Time permitting, topics to be discussed include: (*i*) Basic aspects of ARPES: theoretical concepts and instrumentation; (*ii*) Brief overview of many-body effects and how to study them using ARPES; (*iii*) Electron-phonon coupling (and similar electron-boson couplings); (*iv*) Quasi-1D systems; (*v*) Low- and high-T_C superconductors; (*vi*) Effects of spin-orbit coupling on the electronic structure; (*vii*) 2D electron gases at oxide surfaces and interfaces; (*viii*) Kondo resonance and periodic Anderson lattice; (*ix*) Heavy fermions and exotic phase transitions. Furthermore, as a practical training, we will perform some simple simulations of the spectral function and electronic structure of a few basic systems of importance in correlated-electron physics, such as the Fermi liquid, the Einstein electron-phonon coupling, or the «Marginal Fermi liquid».

Suggested introductory readings (textbook, review or articles)

1. S. Hüfner. *Photoelectron Spectroscopy – Principles and Applications*. Third edition, Springer (Berlin), 2003.
2. S. Hüfner (Editor). *Very High Resolution Photoelectron Spectroscopy*. Lecture Notes in Physics **715**, Springer (Berlin), 2007.
3. F. Reinert and S. Hüfner, New Journal of Physics **7**, 97 (2005).
4. A. Damascelli, Z.-X. Shen, S. Hussain, Rev. Mod. Phys. **75**, 473 (2003).
5. J. C. Campuzano, M. R. Norman, M. Randeria, cond-mat/0209476.
6. J. Braun. *The theory of angle-resolved ultraviolet photoemission and its application to ordered materials*. Rep. Prog. Phys. **59**, 1267-1338 (1996).

Basics of optical spectroscopy studies of superconductors

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[1]Centre de Sciences Nucléaires et de Sciences de la Matière, Université Paris-Sud, Bâtiments 104 et 108, 91405 Orsay cedex, France

Abstract. Optical spectroscopy is a valuable tool to explore the electrodynamics of elementary excitations in the bulk of solids. This lecture will introduce the basic aspects of optical (infrared and visible) spectroscopy and its application to the study of superconductors. We will discuss among others how the technique can be used to study the superconducting gap, the superfluid density, and microscopic aspects of the superconductivity mechanism in high-Tc superconductors.

Suggested introductory readings (textbook, review or articles)

1. M. Dressel and G. Grüner. *Electrodynamics of solids*, Cambridge University Press (Cambridge), 2002.
2. F. Wooten. *Optical properties of solids*, Academic Press (New York), 1972.

Crystallographic and magnetic structures from neutron diffraction: the power of symmetries.

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Abstract. The use of symmetries to understand the properties of matter is a central subject in science, in particular in crystallography and magnetism. Besides, neutron diffraction, combined with group theory, is a privileged tool to determine both a nuclear and a magnetic structure, as described in this lecture. In the first section, the basic concepts of crystallography, based on symmetries, are depicted (point groups, lattice and motif, space groups), with the final aim to be able to read and understand the international tables for crystallography. The reciprocal lattice, required for diffraction, is also introduced. The second section is devoted to the description of magnetic structures (propagation vector, the various magnetic orderings) and to their symmetries (time inversion, magnetic point groups and space groups). In the third chapter, after the description of nuclear and magnetic neutron diffraction (Bragg's law, nuclear and magnetic structure factors, extinction rules), the use of group theory to solve the nuclear and magnetic structures will be exemplified, in the case of both powder and single-crystal diffraction. All these concepts will be illustrated by various chemical compounds shown throughout the whole lecture and by the utilization of useful websites.

Suggested introductory readings (textbook, review or articles)

1. *Contribution of symmetries in condensed matter,* Edited by B. Grenier, V. Simonet, and H. Schober, EPJ Web of Conferences, Volume 22 (2012).
2. *Neutrons and magnetism*, Edited by V. Simonet, B. Canals, J. Robert, S. Petit, and H. Mutka, SNF Collection 13, EDP Science, Volume 13 (2014).

Inelastic Spectroscopy

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[1] *Laboratoire de Physique des Solides, CNRS, Université Paris-Sud, Université Paris-Saclay 91405 Orsay cedex, France*

Abstract. Inelastic spectroscopy is a powerful tool to probe both ground and excited states of all kind of material, including unconventional electronic states. This lecture will be divided into two parts. The first part will consist in an introduction to different spectroscopic techniques using either photon-matter or neutron-matter interaction. We will discuss both neutron [1] and photons [2] scattering and the absorption process and associated emission in the particular case of X-rays. The aim is to provide an overview of the physic involved in theses techniques and what information can be extracted from it (electronic structure, electronic dd excitations, phonons, magnons etc...). We will focus on some mainstream examples relevant in this thematic school of unconventional electronic states. The second part of this lecture will deal specifically with magnetism. As we will see, inelastic measurements can provide crucial information on classical or exotic magnetic ground sates and their associated excitations, namely cristal field, magnon [3], electromagnon [4]... We will see how photon and neutron spectroscopy are complementary (with emphasis on Raman spectroscopy [5], neutron scattering [1] or Resonant Inelastic X-ray Scattering (RIXS) [6]) and will provide a state of the art overview of these experimental techniques.

References

[1] S.W. Lovesey *Theory of Neutron Scattering from Condensed Matter* **(1984)**

[2] K. Hamalainen and S. Manninen *Resonant and non-resonant inelastic x-ray scattering* **Journal of Physics: Cond. Mat. 13 (2001)**

[3] C. Kittel, *Introduction to Solid State Physics* **7th edition (Wiley, 1995)**

[4] S.-W. Cheong and M. Mostovoy *Multiferroics: a magnetic twist for ferroelectricity* **Nature Materials 6, 13 (2007)**

[5] YR Shen N. Bloembergen *Interaction between Light Waves and Spin Waves* **Physical Review 143, 172 (1966)**

[6] L. Braicovich et al. Magnetic Excitations and Phase Separation in the Underdoped $La_{2-x}Sr_xCuO_4$ Superconductor Measured by Resonant Inelastic X-Ray Scattering **Phys. Rev. Lett. 104, 077002 (2010)**

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De la synthèse minérale aux corrélations composition chimique-structure-propriété dans des matériaux d'applications à base d'éléments de transition ou de terres rares.

Panorama en chimie du solide à l'aube du XXIème siècle

Alain Demourgues

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Pour chaque élément de transition ou terre rare (Ti, Fe, Ce) stabilisé dans des oxydes, des chalcogénures ou des intermétalliques, les grandes familles structurales seront décrites en ayant spécifié au préalable les voies de synthèse. La liaison chimique qu'elle soit à caractère ionique, covalente ou métallique sera largement discutée (état d'oxydation, potentiel de Madelung, polarisation, champ cristallin, couplage spin-orbite, hybridation et covalence) et corrélée aux propriétés de réactivité, électronique, ionique, magnétique ou optique. Les trois parties suivantes associées aux trois éléments chimiques, Ti, Fe et Ce feront l'objet de cette présentation de façon à avoir un panorama suffisamment large des voies de synthèse, des grandes familles structurales associées à des propriétés et applications en chimie du solide.

(1) Composés à base de Ti et applications (ferroélectricité, batterie, optique et photocatalyse)
(2) Composés à base de Fe et applications (conductivité ionique/électronique, , optique/pigments, magnétisme, supraconductivité)
(3) Composés à base de Ce et applications (catalyse redox, magnétisme, luminescence et pigments)

Les composés à anions mixtes : synthèse, réseaux cristallins et propriétés électroniques/magnétiques/optiques

Alain Demourgues

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Alors que les oxydes à valences mixtes ont fait l'objet de nombreuses études sur la base d'une famille structurale (perovskite, NaCl) et des propriétés électroniques qui en découlent, les composés associant plusieurs anions d'électronégativité et de polarisabilité variables autour d'un même cation suscitent actuellement un vif intérêt, notamment en raison de la découverte des oxy(fluoro)pnictures à base de fer supraconducteurs (Tc~50 K).

Nous montrerons ainsi les combinaisons judicieuses d'éléments sur la base de la théorie HSAB (dur-dur et mou-mou) pour stabiliser plusieurs anions autour d'un élément de transition ou d'une terre rare mettant en jeu des liaisons concurrentielles autour du métal. Le cas des groupements anioniques tels que carbonates, phosphates ou sulfates associant également d'autres anions sera abordé. Les voies de synthèse seront mises en œuvre compte tenu de la réactivité des anions (oxydes, halogénures, chalcogénures, pnictures, …) mais également de leur électronégativité et de leur polarisabilité. Le principe de construction de la plupart de ces réseaux sera présenté en mettant en jeu d'une part des liaisons à caractère plutôt iono-covalente au sein de feuillets ou blocs et d'autre part des liaisons covalentes voire métallique au sein d'autres couches du réseau leur conférant ainsi un caractère bidimensionnel bien marqué. Une attention toute particulière sera portée sur le polyèdre de coordination du métal mais également de l'anion pour imaginer de nouvelles compositions et structures. Enfin, compte tenu des différences d'électronégativité associées au niveau de Fermi, des évolutions des diagrammes monoélectroniques peuvent être considérées et nous montrerons comment nous pouvons mieux appréhender les instabilités électroniques et magnétiques au sein de ces réseaux à anions mixtes.

Les composés à anions mixtes : synthèse, réseaux cristallins et propriétés électroniques/magnétiques/optiques

Alain Demourgues

[1]*CNRS, Université de Bordeaux, ICMCB, 87 Av du Dr A. Schweitzer. 33608 Pessac Cedex. France*

Alors que les oxydes à valences mixtes ont fait l'objet de nombreuses études sur la base d'une famille structurale (à titre d'exemple : perovskite, NaCl) et des propriétés électroniques qui en découlent, les composés associant plusieurs anions d'électronégativité et de polarisabilité variables autour d'un même cation suscitent actuellement un vif intérêt, notamment en raison de la découverte des oxy(fluoro)pnictures à base de fer supraconducteurs (Tc~50 K).

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Design of metastable phases with novel electronic properties

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Abstract. Extreme thermodynamic conditions, such as high pressures in the GPa range and above, offer the unique opportunity of stabilizing metastable phases with unusual structural and electronic properties [1,2]. For instance, high pressure increases the width of the electronic bands, thus favoring metallic properties, and tends to stabilize structures with high coordination numbers (or high-density). In previous years, these general guidelines have led to the discovery of several novel phases with remarkable properties, such as superconductivity at the surprisingly high temperature of 203 K in H_2S [3], or ultrahard phases [4]. The challenge is an effective search of novel phases with the desired electronic and functional properties. In order to face this challenge, a powerful research strategy is the combination of *ab initio* calculations of the total energy and of the electronic structure with *in situ* probes, such as x-ray diffraction. In this lecture, I shall provide an introduction to the topic by illustrating selected examples of novel metastable phases that have been successfully synthesized under high pressure, such as transition metal oxides with multiferroic properties and transition metal sulfides exhibiting heavy-fermion behavior. I shall also provide an overview on some recent advances in the theoretical and experimental methods used to effectively search for novel phases, with emphasis on *in situ* synchrotron x-ray diffraction.

References

[1] J. V. Badding, Ann. Rev. Mater. Sci. **28**, 631 (1998).
[2] P. F. McMillan, Nature Materials **1**, 19 (2002).
[3] A.P. Drozdov, M.I. Eremets, I.A. Troyan, V. Ksenofontov, S.I. Shylin, Nature **525**, 14964 (2015).
[4] Q. Gu, G. Krauss, W. Steurer, Advanced Materials **20**, 3620 (2008).

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Weak and strong localization in disordered systems

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Within a Boltzmann picture, non-interacting quantum particles in disordered media propagate according to a diffusive motion, which can be interpreted as a random walk through the defects of the material. When the coherence of particles is preserved however, the multiply scattered de Broglie waves interfere destructively. In general this leads to a reduction of the diffusion coefficient, a phenomenon known as weak localization. At strong enough disorder, the diffusion coefficient can even vanish and transport comes to the halt. This is the threshold of Anderson —or strong— localization.

In the lecture, I will first briefly discuss Anderson localization through its historical and phenomenological scaling description, and then present a microscopic approach known as the self-consistent theory of localization. Although approximate, the self-consistent theory is relatively accessible and accurate. It is also very flexible, for instance providing predictions for experimental problems as different as the conduction of electrons in dirty metals, the propagation of photons in complex dielectric structures or the motion of atoms subjected to random optical potentials. A large part of the lecture will be also devoted to the discussion of recent experimental and theoretical developments in the field, as well as of open questions.

Suggested references

1. "Fifty years of Anderson localization", edited by E. Abrahams (World Scientific Press, 2010).
2. E. Akkermans and G. Montambaux, "Mesoscopic Physics of electrons and photons", Cambridge University Press (2007).
3. Dossier Localisation d’Anderson (in French) in Images de la Physique 2009, http://www.cnrs.fr/publications/imagesdelaphysique/2009.htm

Superconductivity: from conventional to exotic

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Abstract. Superconductivity is not a recent phenomenon: It was first observed in 1911. And its first microscopic explanation was formulated by Bardeen, Cooper, and Schrieffer (BCS) in 1957. Nevertheless, it remains a fascinating phenomenon that provides evidence for quantum coherence on a macroscopic scale. And it is also an active field of research with many new emerging concepts. The aim of the lecture will be to give an general introduction to superconductivity, as well as present some of the ideas of ongoing research in this field.
I will start by introducing the phenomenology of superconductivity. I will then present the conventional BCS theory, and show that it allows explaining basic properties of superconducting materials. The BCS theory will be further extended to various kinds of anisotropic pairings. This will allow discussing the basic properties of unconventional, ferromagnetic, non-centrosymmetric, and topological superconductors. A last part of the lecture will address more exotic topics, such as the strong-coupling theory of superconductivity, the crossover to the Bose-Einstein condensation, and the superconductivity of strongly disordered electronic systems.

Many excellent textbooks on superconductivity exist, see for instance Refs. [1–3]. Monographs on unconventional [4], disordered [5], non-centrosymmetric [6], and topological [7] superconductors can also be found.

References

[1] P. G. de Gennes, *Superconductivity of metals and alloys* (Perseus, Cambridge, MA, 1999).
[2] M. Tinkham, *Introduction to superconductivity* (McGraw-Hill, New York, 1996).
[3] A. A. Abrikosov, *Fundamentals of the theory of metals* (Elsevier, Amsterdam, 1988).
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Introduction to Density Functional Theory (DFT)

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Abstract: First-principles approaches to condensed matter consist in starting from what we know about a material, i.e. its chemical composition, and to calculate its energy and properties. In the Born-Oppenheimer approximation, the electrons are the particles setting the many-body problem. Amongst the theoretical methods available to solve this many-body problem, Density Functional Theory (DFT) [1] is the most widely used formalism in condensed matter as it combines numerical efficiency with acceptable accuracy and reliability. It is regarded as the main computational tool to perform electronic structure calculations for periodic systems with a realistic complexity. Within the framework of Kohn–Sham DFT (KS DFT) [2] the intractable many-body problem of interacting electrons moving in a static external potential is reduced to a tractable problem of non-interacting electrons moving in an effective potential $v_{\mathrm{eff}}(\vec{r})$. This formalism will be briefly introduced together with the main classes of energy functionals developed so far to reach an accurate description of $v_{\mathrm{eff}}(\vec{r})$. [3] The strength and weakness of each class of functional will then be discussed in regard to specific material properties.

References:

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[3] A review of the different classes of energy functionals can be found in any textbook dedicated to DFT. Specific references will be given during the school.

Structural Prediction

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Abstract: More than twenty years ago, John Maddox declared that the inability to predict the structure of a crystal from its chemical composition is a "*scandal in the physical sciences*". [1] Ever since, although substantial progress has been made, structural prediction from the only chemical composition remains extremely difficult because of the complexity of the potential energy surface (PES) of a solid that is based on a large number of degrees of freedom. This clearly sets the challenge that has not to be confused with geometry optimization (or structure relaxation) which “simply” requires the knowledge of a starting geometry and a simple local minimization procedure to reach equilibrium structures with reasonable reliability. In contrast, starting from the chemical composition alone and find the minimum of the PES requires global minimization procedures that must go through efficient sampling of the N-dimension PES. To solve this global space-group problem, various algorithms have been developed in the past 10 years. These approaches are based on genetic, [2] Bayesian [3] or stochastic [4] algorithms and begin to be extensively used to discover new materials with targeted properties.

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Practical: Spin waves

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Abstract. Developed in the 1950's [1-5], spin wave theory has been a milestone of magnetism, still of fundamental importance in condensed matter physics to date. Although it is well acknowledged nowadays that it has strong limitations - a number of magnets actually never order, owing to strong quantum fluctuations, low dimensionality or frustration effects - this approach allows a simple treatment of magnetic collective excitations around a mean field long range magnetic order. Using the *SpinWave* software, a general code developed at LLB [6] and able to deal with any magnetic structure, the aim of this practical is to simulate the spin waves spectra in simple cases. The results will be discussed in connection with lectures on magnetic structures, neutron scattering spectroscopy and the general introduction to magnetism in solid state physics.

References

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Topological Aspects of Insulators, Superconductors and Semimetals

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Abstract. Topology is a branch of mathematics that studies properties of objects invariant under smooth deformations. It allows to define topological invariant that characterizes objects that can be deformed into each other. Examples of such invariants include the winding of curves or the Euler index of two dimensional surfaces. In the context of condensed matter, topology allows to characterizes robust properties of vector fields. The first example includes the description of defects of an order parameter fields : vortices, dislocations, disclinations, etc. More recently, topology has been used to describe the properties of an ensemble of abstract vectors describing the quantum states of particles in a gapped phase, or a semi-metallic phase. In these examples, the vectors belong to a Hilbert space, and are parametrized by a quasi-momentum belonging to the first Brillouin zone. These ensemble of vectors define the ground state of the phase we consider. In these lectures I will describe the basic idea being the topological characterization of these vectors fields. I will then discuss the manifestation of these topological properties as edge or surface states. I will give a particular emphasis on superconductors, building on the other lectures of the school by M. Houzet for the fundamental aspects. I will also describe the properties of semi-metallic phases, which can be viewed as topological defects of these vector fields, but in the Brillouin zone. The practical session will be devoted to the study of simple models and the numerical determination of their topological property.

There already exists several good review articles and books on topological properties of phases, listed below. The book by A. Bernevig is particularly recommended.

References

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Correlated Electron Materials – A Playground for Electronic Structure Theory

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Abstract. The field of electronic structure calculations for correlated materials has witnessed tremendous progress in recent years due to the development of combined electronic structure and many body theories. We will give an introduction to the concept of electronic correlations and the modeling thereof. Focussing on excited states properties, we will point out the need of going beyond band theory for correlated materials. We will summarize some of the main strategies of many-body theory and their combination with realistic electronic structure techniques. In particular, we will describe the ideas and formalism of dynamical mean field theory, and discuss its application in the electronic structure context. Finally, we will comment on current questions in the field and open challenges.

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Topological quantum phase transition in the Ising-like antiferromagnet $BaCo_2V_2O_8$

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Abstract.
In the present study, we show by a combination of neutron scattering experiments, numerical calculations and field theory that a topological quantum phase transition occurs in the Ising-like spin chain compound $BaCo_2V_2O_8$ when subjected to a magnetic field transverse to the Ising axis (which points along the chains) [1].

References

[1] Q. Faure *et al.* , arXiv:1706.05848

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