Research Networking Programmes

Science Meeting – Scientific Report

The scientific report (WORD or PDF file - maximum of seven A4 pages) should be submitted online within two months of the event. It will be published on the ESF website.

***Proposal Title**: Theoretical Spectroscopy Lectures*

Application Reference N°: 5712

1) Summary (up to one page)

The aim of the school was to give a deep introduction on the theoretical and practical aspects of the electronic excitations. Electronic excitations are probed by experimental techniques such as optical absorption, EELS and photo-emission (direct or inverse). From the theory point of view, excitations and excited state properties are out of the reach of density-functional theory (DFT), which is a ground-state theory. In the last twenty years other ab-initio theories and frameworks, which are able to describe electronic excitations and spectroscopy, have become more and more used: time-dependent density-functional theory (TDDFT) and many-body perturbation theory (MBPT) or Green's function theory (GW approximation and Bethe-Salpeter equation BSE). In fact, computational solutions and codes have been developed in order to implement these theories and to provide tools to calculate excited state properties. The present school focused on these points, covering theoretical, practical, and also numerical aspects of TDDFT and MBPT, and codes implementing them (ABINIT, DP, EXC).

2) Description of the scientific content of and discussions at the event (up to four pages)

The presentation of the theory and theoretical aspects of the implementation took place in the morning sessions. The afternoon sessions were devoted to practical hands-on of the theory studied in the morning: DFT with Abinit (Day 1), TDDFT with DP (Day 2), GW with Abinit-GW (Day 3 and 4), Bethe-Salpeter with EXC (Day 5). A more detailed description of the lectures follows

- **Introduction to spectroscopy: In this lecture, we described various experimental techniques used to investigate the spectroscopic properties of matter. At first a presentation of the processes (scattering, absorption, and emission) resulting from the interaction of particles with matter, and which are involved in those experimental techniques (photoemission spectroscopy (PES), inverse photoemission spectroscopy (IPES), x-ray absorption spectroscopy (XANES, EXAFS, and XANES), electron energy loss spectroscopy (EELS), inelastic x-ray scattering spectroscopy (IXS), reflectance anisotropy spectroscopy (RAS), Auger electron spectroscopy (AES), and X-Ray fluorescence spectroscopy (XRF)). For all methods, a link has been given to the quantities that can be computed using the theoretical methods in the subsequent lectures.**
- **Micro-Macro connection: One hour lecture on the connection between the measurable quantities (macroscopic) and calculated quantities (microscopic). This lecture is crucial, for this connection is never well explained in textbooks or articles.**
- **Density-Functional Theory: This two-hour lecture covered the basics of density-functional theory : formalism and implementation. A special care was taken to present the shortcomings of Density Functional Theory as concerns its use for the computation of band structure, and, on the other hand, its usefulness as a starting point for more elaborate theories. The hands-on sessions were also prepared. The following sections were covered: The electronic N-body problem, Functionals of the density, The Kohn & Sham approach, Density Functional Theory : approximations, The band gap problem, The plane wave basis set / Brillouin zone integration, Pseudopotentials, Computing the forces, Iterative algorithms, ABINIT**
- **Introduction to TDDFT: A review of time-dependent density-functional theory and its fundamental assumptions, theorems, caveats and drawbacks has been presented. In particular, we have illustrated the Linear-Response TDDFT in an actual implementation which is in Frequency-Reciprocal space and on a Plane-Waves basis, as implemented in the DP (Dielectric Properties, http://www.dp-code.org) code. This scheme is well suited to EELS and optical spectroscopy calculations, and particularly convenient for infinite periodic bulk solids, but also semi-infinite systems like surfaces, wires and tubes by the use of supercells. A critical analysis of all the classical approximations (RPA, Adiabatic LDA, with and without local-field effects) as well as the most recent ones (long-range contribution only, Nanonoquanta kernel, etc.) has been presented together with illustrating examples of spectra on prototype condensed matter systems, like bulk silicon, graphite, nanotubes, etc. This lecture was followed by a practical session on the use of DP code.**
- **Many-Body Perturbation Theory: In this lecture, we presented the theoretical basics required to introduce the GW approximation of the many-body problem. The GW approximation has been shown to be very successful in predicting the band gaps of solids. It improses significantly over the standard density-functional approaches for the electronic structure. I introduce the so-called Hedin's equations, which offer an exact formulation of the many-body problem in a functional language. The central quantities are the Green's function G and the screened Coulomb interaction W. In this framework, the GW approximation appears naturally as a first order approximation in the "small" quantity W. This is a formal derivation of the GW approximation. In order to elucidate the physical content of the GW approximation, we show that the GW approximation is a**

natural improvement over the well-known Hartree-Fock scheme. The only difference comes from the screening of the Coulomb interaction, which accounts for the fact that the interaction between electrons in a solid is decreased by the polarization of the medium.

- **Post-processing tools and automatisms: This year we decided to include a new lecture: the GW calculations are becoming more and more standard, also helped by the computational power increase. However converging a GW calculation is far from being trivial, for many parameters have to be adjusted at the same time. Python post-processing tools can permit to efficiently do that, together with the construction of converging databases, which will reveal useful for other scientists (also it improves the reproducibility of numerical results).**
- **Bethe-Salpeter Equation: This lecture presents the Many-Body approach for the description of polarizability. Within the Green's functions formalism, the linear response polarizability is given by the 2-particle Green's function which obeys to a Dyson-like equation, similarly to the linear response TDDFT eqution. The derivation of the Bethe-Salpeter Equation as well all the approximations involved in the (several) steps are illustrated in this two-hour lectures, before presenting the numerical aspects useful for the afternoon hands-on.**

3) Assessment of the results

From the organizers' point of view the school has been a frank success. Thanks also to the cumulated experience of last editions, and to a good team-work among tutors, the lectures have been largely considered appropriate in length, complexity and clarity, by the students. The participation level has always been very high, and we have been glad to notice how, sometimes, the discussion time has been stretched much over the allocated time, in particular for the most sensible lectures (MBPT and TDDFT).
Incidentally none of the tutors used the upstairs room dedicated to them, in order to privilege a continuous availability to the students.
All participants attended the social dinners.
No problems have been encountered in this school, while the organization and the connection with Guy, Marianne, Bogdan and Nathalie (thanks for letting us feel most welcome) was flawless.
Given this, and previous, success of the school, we are going to apply for a very similar tutorial in 2017.

4) Annexes 4a) and 4b): Programme of the meeting and full list of speakers and participants

Annex 4a: Programme of the meeting

Day 1 - May, 18th 2015

Introduction to Spectroscopy

Micro-macro connection

Caffeine break

Density Functional Theory

Lunch

DFT hands-on with Abinit

Social Dinner

Day 2 - May, 19th 2015

Time Dependent Density Functional Theory

Caffeine Break

Time Dependent Density Functional Theory

Lunch

TDDFT Hands-on with DP

Day 3 - May, 20th 2015

Many-Body Perturbation Theory

Caffeine Break

GW approximation

Lunch

Discussion - catch up – Q andA

Day 4 - May, 21st 2015

GW in practice

Coffee Break

Post-processing and tools

GW hands-on with Abinit

Lunch

GW hands-on with Abinit

Day 5 - May, 22nd 2015

Bethe-Salpeter Equation

Caffieine Break

BSE hands-on with EXC

Lunch

BSE hands-on with EXC

Annex 4b: Full list of speakers and participants

Organizers
Valerio OLEVANO France, CNRS Institut Neel, Grenoble
Gian-Marco RIGNANESE Belgium, Université Catholique de Louvain
Francesco SOTTILE France, Ecole Polytechnique, Palaiseau

Tutors
Matteo GATTI France, Ecole Polytechnique
Michiel VAN SETTEN Belgium, Universite Catholique de Louvain
Matteo GIANTOMASSI Belgium, Universite Catholique de Louvain
Valerie VENIARD France, Ecole Polytechnique, Palaiseau

Participants
Victor DA SILVA SANTANA Brazil, Federal University of Bahia/University
Eitam ARNON Israel, The Hebrew University of Jerusalem
Marc BARBRY Spain, Materials Physics Center
Paolo BONARDI Italy, University of Milan
Sven BORGHARDT Germany, Jülich Research Centre
Pedro BORLIDO Germany, Friedrich Schiller University
Yael CYTTER Israel, Hebrew university of Jerusalem
Nicolas DARDENNE Belgium, Université Catholique de Louvain
Francesca DELCHIARO Italy, University of Parma
Yuzheng GUO United Kingdom, University of Cambridge
Anh HA Belgium, Université Catholique de Louvain
Tetiana KHOTIAINTSEVA France, Ecole Polytechnique, Palaiseau
Alberto MARMODORO Germany, Max Planck Institute of Halle
Sriram POYYAPAKKAM RAMKUMAR Belgium, Université catholique de Louvain
Gianluca PRANDINI Switzerland, Swiss Federal Institute of Lausanne
Lucie PRUSSEL France, Ecole Polytechnique, Palaiseau
Carlos RODRIGUEZ FERNANDEZ Spain, University of Valencia
SOMANANDA SANYAL Italy, University of Parma
Marilena TZAVALA France, Ecole Polytechnique, Palaiseau
Gil VANDER MARCKEN Belgium, Université catholique de Louvain
Marco VANZINI France, Ecole Polytechnique, Palaiseau
Vojtech VLCEK Israel, Hebrew University of Jerusalem
Martin ZELENY Czech Republic, Brno University of Technology