Tutorial Scientific Report

Please do not repeat the program (unless there were last-minute changes) or the initial description - we already have this material.

Title	Theoretical Spectroscopy Lectures: Theory and Codes
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Aim(s) of the Tutorial (one-two paragraphs)

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).

Report on key lectures and hands-on sessions (one page)

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 and Day 3), TDDFT with DP (Day 2 and Day 3), GW with Abinit-GW (Day 4), Bethe-Salpeter with EXC (Day 5). Afternoon session 3 (on Wednesday) was considered free, however most of the students stayed in the computer room, working on the previous days' assignmentstracts 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.

• 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 foundamental 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) 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.

• 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 equation. 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.

Report on the feedback from the "students" (one paragraph at least)

We haven't had any official feedback (maybe Cecam has), only warm appreciation given to us by all students during this 5-days tutorial. The most welcome part of the tutorial was indeed the the concept, hard theory in the morning, immediately followed by the hands-on on the code. This is particularly important on a theory like GW, where an important researcher input is demanded (no black box GW code so far), but it is true also for TDDFT and Bethe-Salpeter. Students (and tutors) were also pleased of the new location at Cecam that permitted us to stay focused all along the week, with everything in place (conf room, computer room, management and secretarial staff).
Finally at the specific request about which part of tutorial they preferred, there was a consensus about the crucial need of many-body training. Some of the students had participated in events concerning TDDFT, while a coherent, complete training on MBPT was missing in their opinion, and for this reason the 3 days dedicated to MBPT in this school were highly appreciated. For this reason we are going to present a different, though very similar, tutorial for the 2012 season more centered on many-body theory and applications, on both spectroscopy and (timely novelty) quantum transport.

Do you have suggestions for new related tutorials?

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). Almost none of the students took the Wednesday afternoon free, preferring a discussion with the lecturers or continuing the hands-on in his/her own account. 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 dinner.
No problems have been encountered in this school (with the small exception of the missing mount points of the nfs disks on Day 1, immediately solved by Bogdan), while the organization and the connection with Emilie, Marianne, Bogdan and Wanda (thanks for letting us feel most welcome) was flawless.
Given this, and previous, success of the school, we are going to apply for a slightly changed (but same in spirit) tutorial in 2012.