

Theory days Stochastic and Dissipative effects

Nov-Dec 30, 1, 2, 2011

IRSAMC
Toulouse

Multi-ionization
Photodissociation
Time dependent DFT
Surface hopping
Nonadiabatic effects



CoDFT



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THEORY DAYS ON STOCHASTIC AND DISSIPATIVE EFFECTS IN AB INITIO METHODS

TOULOUSE, NOVEMBER 30 TO DECEMBER 2, 2011

1 Aim and objectives

Following the tradition of the previous successful two meetings (2009 and 2010), the Workshop aims to stimulate constructive discussions, collaborations, and knowledge exchange among a selected group of theoreticians. This year the workshop will be devoted to the ab initio description of Stochastic and Dissipative effects in real time dynamics. The typical physical situations we aim to describe concern in particular the irradiation of clusters and molecules by extreme light. By extreme light we mean in particular high intensity lasers for which energy deposit is known to be especially important. But other "extreme" light sources such as FEL or attosecond lasers certainly also constitute highly interesting cases to explore. Real time dynamics simulation is a valuable resource to the chemical and physical communities, since it allows for direct mimicking of numerous time-domain experiments and provides a detailed atomistic description of chemical and physical processes and interactions. However, in order to make the simulation feasible one has to recur to some approximations, on which the accuracy of the results rely. We will focus on how to reproduce realistic situations such as photodissociation or multi-ionization within state-of-the-art methodologies such Time-dependent Density-Functional Theory (TDDFT). Attention will be paid to the failures of the current approximations and on how to improve. Approaches beyond TDDFT, such as Time-Dependent Density Matrix, stochastic TDDFT and Trajectory Surface Hopping methods will be also discussed.

We plan to gather people from various groups working in this domain, mostly in western Europe. The workshop is intended to be a working forum, thus rather informal. The format will consist in a series of long detailed talks, typically 1 hour (40 mn talk + 20 mn for questions) focusing in particular on ongoing problems and open ends. Some free time will furthermore be reserved for collective discussions. We thus urge participants to prepare their talks in this spirit. Ultimately a most efficient organization would consist in having a limited number of talks per representative group in order to avoid doublings.

If a consensus is reached during the workshop it would be highly profitable to envision a sequel to this workshop in order to possibly establish, at best collaborative

links between the various groups with possible exchange of researchers and students, at worst an ongoing follow up of progress in the field.

2 Scientific program

The detailed program will be prepared as soon as possible after replies from participants.

We plan to start the workshop on a Wednesday just after lunch and end it on the following Friday early afternoon. This would allow participants to reach Toulouse in the Wednesday morning and be back home in the Friday evening.

A tentative program is thus :

Day 1 (Wed) : 14 :00 - 17 :30 (3 × 1 hour + 1 coffee break)

Day 2 (Thu) : 08 :30 - 13 :00 (4 × 1 hour + 1 coffee break)

Day 2 (Thu) : 14 :30 - 18 :00 (3 × 1 hour + 1 coffee break)

Day 3 (Fri) : 08 :30 - 13 :00 (4 × 1 hour + 1 coffee break)

Day 3 (Fri) : possibly a short final session in the afternoon.

3 Practical aspects

3.1 Registration and lodging

As in 2009 and 2010 there will be no registration fee. We shall cover lodging, meals, and local transportation for about 15 participants during the duration of the workshop (arrival Nov 30, departure Dec 2), on the basis of first confirmed, first served.

Participants will be lodged in hotels downtown Toulouse at walking distance from major metro stations along line B. There is a direct metro line (line B) connecting downtown to university. Travel takes about 20 minutes with trains every few minutes (less than 5 mn).

Meeting will take place at IRSAMC in the university Campus : for a map, see <http://www.irsamc.ups-tlse.fr/index.php?lien=venir>

3.2 Access to Toulouse

Airports

Toulouse airport is connected to major west European airports and hubs (Paris Orly and Roissy Charles de Gaulle, Munich, Frankfurt, London, Amsterdam) with regular connections by Air France/KLM, Lufthansa, British Airways for the major companies and also with connections by (Low Cost) Easy Jet. Plane provides by far the simplest access to Toulouse with reasonable fees for sufficiently early booking.

<http://www.toulouse.aeroport.fr/>

There is a shuttle to downtown (first stop at Compans Caffarelli, on line B of metro) every 20 mn (cost is 5 euros one way, 8 euros return trip); for details, see <http://www.toulouse.aeroport.fr/fr/aeroport/acces-plans-parkings/acces/se-deplacer-en-transport-en-commun>

As soon as one catches the shuttle, it takes about half an hour to get to the University thanks to the connection with line B at Compans Caffarelli station.

An alternative access is provided by Carcassonne airport (about 45 minutes by car from Toulouse) which has a Low Cost access through Ryanair

<http://www.carcassonne.aeroport.fr/>

In case of major problem, we shall organize some transfer. It would be useful to know sufficiently in advance such details.

Train

Central station is Toulouse Matabiau connected to line A of metro (see below) and is connected to major french cities.

<http://www.gares-en-mouvement.com/gare.php?gare=frxyt>

Metro

Metro and bus connections (general) : <http://www.tisseo.fr/se-deplacer/horaires>

line A (train station to downtown) :

http://www.tisseo.fr/sites/default/files/Tisseo_hivMETROweb.pdf

line B (downtown to university) :

http://www.tisseo.fr/sites/default/files/Tisseo_hivMETROweb.pdf