11th Nanoquanta Workshop on Electronic Excitations:

A decade of applications of the Bethe-Salpeter Equation
Houffalize, September 19-22 2006

Organizers:
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Gian-Marco Rignanese ❖ Patrick Rinke
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ETSF

Nanoquanta
Network of Excellence

Nanoquanta series of workshops

10th Nanoquanta Workshop on Electronic Excitations:
40 Years of the GW Approximation for the Electronic Self-Energy: Achievements and Challenges
Bad Honnef (Germany) [12-15 September 2005]

9th Nanoquanta Workshop on Electronic Excitations:
Theory and Modeling of Electronic Excitations in Nanoscience
Maratea (Italy) [19-23 September 2004]

8th Nanoquanta Workshop on Electronic Excitations:
Ab initio Electrons Excitations Theory: Towards Systems of Biological Interest
San Sebastián (Spain) [21-24 September 2003]

7th Nanoquanta Workshop on Electronic Excitations:
Ab initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials
Lyon (France) [23-25 September 2002]

6th Nanoquanta Workshop on Electronic Excitations:
Excited states and electronic spectra
Lyon (France) [20-22 July 2000]

5th Nanoquanta Workshop on Electronic Excitations:
Calculation of Electronic Excitations in Finite and Infinite Systems
Lyon (France) [1-3 September 1999]

4th Nanoquanta Workshop on Electronic Excitations:
Spectroscopy of Electronic Excitations in Materials
Valladolid (Spain) [7-9 September 1998]

3rd Nanoquanta Workshop on Electronic Excitations:
Electronic Exchange and Correlation in Advanced Materials
Lyon (France) [11-12 September 1997]

2nd Nanoquanta Workshop on Electronic Excitations:
Electronic Exchange and Correlation in Advanced Materials
Palaiseau (France) [26-28 September 1996]

1st Nanoquanta Workshop on Electronic Excitations
Rome (Italy) [September 1995]

11th Nanoquanta Workshop on Electronic Excitations:
A decade of applications of the Bethe-Salpeter Equation
Houffalize (Belgium), 19-22 September 2006

Scientific Report

The workshop gathered 114 participants from leading international groups. There were 39 oral presentations (17 invited speakers and 22 contributed talks) and 30 posters. The workshop allowed the participants to discuss the advances in the theoretical and computational treatment of optical and dielectric spectroscopy in the framework of many-body-perturbation-theory (MBPT).

Invited speakers from leading international groups gave an in-depth overview of current research activities in MBPT (and related fields) and placed recent results into context. Young researchers (Ph.D. students and post-docs) also had the opportunity to present their work (more than half of the oral presentations were given by non-permanent researchers).

A special emphasis was placed on the assessment of ten years of the Bethe-Salpter Equation (BSE) method presenting its achievements and developments [Session I], applications [Session II], advantages and drawbacks in comparison to the more recent developments of time-dependent density-functional theory (TDDFT) [Session IV & V]. Very interesting discussions took place on the complementarity of the two methods and on the future of BSE with respect to TDDFT.

The state-of-the-art implementations of these *ab initio* methods into existing numerical codes was presented in this meeting. In the same session, an invited speaker described the most recent experimental advances in the field [Session III].

A session was also devoted to the calculation of excited states using Quantum Monte Carlo simulations [Session VI]. Despite the recent advances which have been presented, the method still remains very demanding in terms of computer time.

A series of presentations focused on quantum transport [Session VII] which is an emerging field of computer simulations and whose importance is increasing in the MBPT community. Indeed, the Green's functions

formalism at the heart of MBPT is also particularly well suited to describe electronic quantum transport. Currently, it is used both in the Landauer-Büttiker approach and in the non-equilibrium Green's functions (NEGF) theory, also known as Keldysh formalism. Approaches based on TDDFT have also been presented in this session.

A session was devoted to the latest results obtained in the framework of "Optimized Effective Potentiel" (OEP) within density-functional theory [Session VIII]. It was followed by a series of presentations of applications to surfaces and nanostructures [Session IX]. The last session [Session X] focussed on applications of MBPT.

The poster session gave rise to very interesting discussions. Indeed, wide variety of subjects were being presented and the discussions went well beyond these subjects. The meeting provided an informal atmosphere for stimulating discussions between researchers working in this exciting field. New collaborations were initiated following these discussions.

The presentations were collected (a few are still missing) and are available on the conference website. They will be very useful for both the participants and those people in the field that did not have the opportunity to attend the meeting. In particular, the review talks may also be used as a starting point to enter the field.

It is important to note that the development of theory and codes to simulate optical and dielectric spectroscopy is of great interest not only for research but also for industry. And, the presence of representative of Atomistix, a private companies selling software for high-tech industries, is significant in this view. It is clear that such theory and codes are needed upstream to help solving technical problems. For instance, some of the talks were applications directly connected to actual technological issues.

In this framework, this workshop was very relevant. On the one hand, it helped increasing the collaborations (in order to develop theory and codes) between the various actors of the field. On the other hand, it contributed to the development and the spread of the know-how.

Hereafter, we have attached the conference program. As mentioned above, the presentations and the abstracts are also available on the conference website: http://www.pcpm.ucl.ac.be/etsf/nq06

Tuesday 19		Wednesday 20	
	SESSION I		SESSION IV
09:00	Welcome	09:00	M. Casida
09:10	G. Onida	09:30	S. Ogut
09:50	E. Shirley	10:00	O. Butriy
		10:20	H.-C. Weissker
10:30	Coffee Break	10:40	Coffee break
	SESSION II		SESSION V
11:00	C. Ambrosch-Draxl	11:10	I. Tokatly
11:30	C. Spataru	11:40	L. Reining
12:00	O. Pulci	12:10	E. Räsänen
12:30	Lunch	12:30	Lunch
	SESSION III		SESSION VI
14:30	S. Huotari	14:30	C. Filippi
15:10	J. Sjakste	15:00	P. Umari
15:30	Y. Pouillon		
15:50	Coffee Break	15:30	Coffee Break
	POSTER SESSION		NETWORK MEETING
16:20	Poster Presentations	16:00	Rosella Palomba
16:45	Poster Session	16:30	Meeting
18:30	Dinner	18:30	Dinner

Thursday 21

	SESSION VII (part 1)
09:00	R. Gebauer
09:30	S. Kurth
10:00	K. Thygesen
10:30	Coffee Break
	SESSION VII (Part 2)
11:00	H. Mera
11:20	P .Darancet
11:40	Peter Bokes
12:05	C.-O. Almbladh
12:30	Lunch
	SESSION VIII
14:30	F. Della Sala
14:50	M. Grüning
15:10	S. Sharma
15:30	Coffee Break
	SESSION IX
16:00	L. Ramos
16:25	F. Iori
16:45	D. Varsano
17:05	Break
17:15	K. Gaal-Nagy
17:35	A. Incze
17:55	A. Schindlmayr
18:30	Dinner

Friday 22

	SESSION X (Part 1)
09:00	R. van Leuween
09:40	P. Garcia-Gonzales
10:10	R. Gomez-Abal
10:30	Coffee Break
	SESSION X (Part 2)
11:00	M. Stankovski
11:20	R. Shaltaf
11:40	V. Zhukov
12:00	Farewell
12:30	Lunch

SESSION I : Bethe-Salpeter Equation

(Chair : Patrick Rinke)

9:00 **Welcome**

9:10 **Giovanni Onida** (30'+10')
The Bethe-Salpeter equation and ab-initio calculations:
from the first adventure to a well established tool

9:50 **Eric Shirley** (30'+10')
Progress in GW/Bethe-Salpeter Calculations:
what do we know, what do we not know?

10:30 **Coffee Break**

SESSION II: BSE applications

(Chair : Friedhlem Bechstedt)

11:00 **Claudia Ambrosch-Draxl** (25'+5')
The Bethe Salpeter Equation applied to organic semiconductors:
a critical review

11:30 **Catalin Spataru** (25'+5')
Excitons and their radiative lifetime in semiconducting nanotubes

12:00 **Olivia Pulci** (25'+5')
Electronic and Optical properties of surfaces:
ab-initio calculations within MBPT and TDDFT approaches

12:30 **Lunch**

SESSION III : From experiment to codes via theory

(Chair : Gian-Marco Rignanese)

14:30 **Simo Huotari** (30'+10')
Inelastic x-ray scattering in studies of electronic excitations

15:10 **Jelena Sjakste** (15'+5')
Ab initio calculation of the excitonic linewidth due to electron-phonon interaction in semiconductors

15:30 **Yann Pouillon** (15'+5')
Software integration and development within Nanoquanta

15:50 **Coffee Break**

POSTER SESSION

16:20 **Poster Presentations**

16:45 **Poster Session**

18:30 **Dinner**

SESSION IV: Time-dependent density-functional theory

(Chair : John Rehr)

9:00 **Mark Casida** (25'+5')
Polarization Propagator Corrections to Linear Response Time-Dependent Density-Functional Theory for Molecules with Closed- and Open-Shell Ground States

9:30 **Serdar Ogut** (25'+5')
Is Nano that Different from the Bulk?

10:00 **Olena Butriy** (15'+5')
Electron-nuclear interaction from Time-Dependent Multi-component Density Functional Theory

10:20 **Hans-Christian Weissker** (15'+5')
Dielectric Function of Silicon for Finite Momentum Transfer Signatures of Short-Range Many-Body Effects

10:40 **Coffee break**

SESSION V: TDDFT vs BSE

(Chair : Rodolfo Del Sole)

11:10 **Ilya Tokatly** (25'+5')
Bethe-Salpeter equation from TDDFT perspective: Diagrammatic representation of the exchange-correlation kernel

11:40 **Lucia Reining** (25'+5')
Many-Body Perturbation Theory and Density-Functional approaches: successful combinations

12:10 **Esa Räsänen** (15'+5')
Control of electronic currents by laser in quantum rings

12:30 **Lunch**

SESSION VI: Quantum Monte Carlo

(Chair : Francesco Sottile)

14:30 **Claudia Filippi** (25'+5')
Excitations in (bio)molecules from quantum Monte Carlo

15:00 **Paolo Umari** (25'+5')
Linear and non-linear dielectric response of
periodic systems from quantum Monte Carlo

15:30 **Coffee Break**

NANOQUANTA General Network Meeting

16:00 **Rosella Palomba**, invited speaker from IT4 (25'+5')
Gender Issues

16:30 **Meeting**

18:30 **Dinner**

SESSION VII : Quantum Transport (Part 1)

(Chair : Carl-Olof Almbladh)

9:00 **Ralf Gebauer** (25'+5')
Quantum kinetic simulations of electron transport in nanosystems

9:30 **Stefan Kurth** (25'+5')
An Approach to Quantum Transport Using Time-Dependent Density Functional Theory

10:00 **Kristian Thygesen** (25'+5')
Non-equilibrium GW approach to electron transport in nanoscale contacts

10:30 **Coffee Break**

SESSION VII : Quantum Transport (Part 2)

(Chair : Rex Godby)

11:00 **Hector Mera** (15'+5')
Non-local self-energies in quantum transport calculations

11:20 **Pierre Darancet** (15'+5')
GW description of Correlation effects in Quantum transport on real systems

11:40 **Peter Bokes** (20'+5')
Dynamics of electrons and ab-initio modeling of quantum transport

12:05 **Carl-Olof Almbladh** (20'+5')
Classical Nuclear Motion in Quantum Transport

12:30 **Lunch**

SESSION VIII: DFT OEP band gap

(Chair : Xavier Gonze)

14:30 **Fabio Della Sala** (15'+5')
Kohn Sham gaps, potentials and excitation energies of finite systems using effective exact exchange-correlation potentials

14:50 **Myrta Grüning** (15'+5')
The effect of nonlocality on the band gap within DFT

15:10 **Sangeeta Sharma** (15'+5')
Non-collinear magnetism within OEP with a view to spin dynamics

15:30 **Coffee Break**

SESSION IX: Optical properties applications: surfaces and nanostructures

(Chair : Ludger Wirtz)

16:00 **Luis Ramos** (20'+5')
Additional many-body effects in the absorption spectra of Si nanocrystallites

16:25 **Federico Iori** (15'+5')
Optical Spectra of doped Silicon Nanocrystals

16:45 **Daniele Varsano** (15'+5')
Exciton localisation of quasi 1D systems and optical properties

17:05 **Break**

17:15 **Katalin Gaal-Nagy** (15'+5')
Electronical and optical properties of the Si(113)-3x2 ADI surface: An ab initio study

17:35 **Andrei Incze** (15'+5')
Ab initio study of optical spectra for oxidized Si(100) surfaces

17:55 **Arno Schindlmayr** (15'+5')
Electronic Properties of Point Defects at the GaAs(110) and InP(110) Surfaces

18:30 **Dinner**

SESSION X : MBPT and GW applications (Part 1)

(Chair : Ulf von Barth)

9:00 **Robert van Leuween** (30'+10')
Propagation of the the Kadanoff-Baym equations
for many-electron systems

9:40 **Pablo Garcia-Gonzales** (25'+5')
Many-body and TDDFT methods for total energy calculations

10:10 **Ricardo Gomez-Abal** (15'+5')
An all-electron GW code based on FP-(L)APW+lo:
the role of core electrons

10:30 **Coffee Break**

SESSION X : MBPT and GW applications (Part 2)

(Chair : Valerio Olevano)

11:00 **Martin Stankovski** (15'+5')
Local and non-local vertex corrections in GW for extended
and localised systems

11:20 **Riad Shaltaf** (15'+5')
First Principle Calculations of Band Offsets of SiO2
and ZrSiO4 with Silicon

11:40 **Vladen Zhukov** (15'+5')
The first-principle LMTO+U+SO+GW+T approach
for the calculations of dynamic spin succeptibilities and life-times
of excited electron in metals

12:00 **Farewell**

12:30 **Lunch**

POSTER SESSION

P01. **Hakim Amara**
How to identify defects in carbon nanotubes : STM study and vibrational properties

P02. **Claudio Attaccalite**
Effect of impurities on the optical properties of BN nanotubes

P03. **Silvana Botti**
Identification of CdSe fullerene-based nanoparticles from optical spectroscopy calculations

P04. **Damien Caliste**
A visualisation tool : V_Sim

P05. **Giancarlo Cappellini**
Electronic excitations of oligoacenes in four different charge states: -1, 0, +1 and +2

P06. **Lucia Caramella**
Optical properties of oxidized Si(100)(2x2) surface and local fields contributions on electron energy loss spectrum

P07. **Alberto Castro**
Time-dependent electron localisation function: A tool to visualise and analyse ultrafast processes

P08. **Marco Cazzaniga**
Study of the small-q contribution to the polarizability and the intraband term: from the jellium to the periodic solid

P09. **Letizia Chiodo**
Thiol adsorption effects on Au(111) work function

P10. **Christoph Friedrich**
All-Electron GW Approximation
in the Augmented-Plane-Wave Basis-Set Limit

P11. **Juergen Furthmueller**
Single-particle excitation energies starting
from generalized Kohn-Sham schemes

P12. **Viviana Garbuio**
Excited states of formamide in water

P13. **Matteo Gatti**
Nonlocality and frequency dependence of effective potentials

P14. **Matteo Gatti**
Electronic excitations in Vanadium Oxide (VO2)

P15. **Christine Giorgetti**
Ab Initio calculations of graphene like systems

P16. **Ralf Hambach**
Anisotropy in EEL-spectra for large momentum transfer

P17. **Paula Havu**
Finite Element Implementation of Green's Function Method
for Transport Problems in Nanostructures

P18. **Nicole Helbig**
Towards a reduced density matrix functional theory for solids

P19. **Conor Hogan**
Optical properties of the Sb-stabilized GaSb(001) surface

P20. **Andrew Morris**
Vertex corrections in localised and extended systems

P21. **Tapio Rantala**
Photoexcitation of Disperse Red 1: Comparison of Approaches

List of posters

P22. **Xinguo Ren**
LDA+DMFT computation of the electronic spectrum of NiO

P23. **Claudia Roedl**
Modifications of BSE Due to Spin Polarization:
Antiferromagnetic MnO

P24. **Ersoy Sasioglu**
Magnetic phase diagram of the Mn-based Heusler alloys
from first-principles

P25. **Valerie Véniard**
Second order harmonic generation in crystalline semiconductors

P26. **Claudio Verdozzi**
Entanglement in Anderson Nanoclusters

P27. **Claudio Verdozzi**
Magnetic field effects on optical and transport properties
in InAs/GaAs quantum dots

P28. **Matthieu Verstraete**
The GW space-time formalism at finite temperatures

P29. **Ludger Wirtz**
Electronic excitations in hexagonal layered systems (C and BN)

P30. **Zeila Zanolli**
Ab initio calculation of structural and electronic properties
of InAs and GaAs having wurtzite crystal structure