REPORT ON ESF SUMMER SCHOOL
AB-INITIO MANY BODY THEORY
JULY 22-28, 2007
SAN-SEBASTIAN, SPAIN

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Aims:

The School on Ab-initio Many Body Theory is in response to very recent developments. The aim is here to understand electronic correlation effects on an ab-initio basis, by starting from realistic wave functions obtained from density functional calculations, leading to a material-specific description of many body effects. The School will reflect the strong progress in this field.
The lectures review the whole field, as well as discuss latest results. The program consists of a good balance between theoretical and experimental lectures, as well as contributions from industry.
The list of topics include:

- Basic density functional theory (DFT) and Time-dependent DFT.
- New experimental techniques for excitation spectrum of materials Many-body theory
- Physics of correlated materials - theory and experiments.
- Basic of Quantum Monte Carlo and Quantum chemical methods.
- Combining the best of different worlds: MBPT-GW-DMFT and TDDF.
- Selected Applications.

The summer school will have a poster session where the young researchers will be able to present their work.
The aims are:

- To review the present state of the art and understanding.
- To give an overview on theoretical and experimental research methods.
- To give a perspective of the future development of the field.
- To discuss the possible technological applications.

In collaboration with Marie Curie series of events programme "Psi-k Training in Computational Nanoscience", Nanoquanta Network of Excellence "European Theoretical Spectroscopy Facility (ETSF)", European Science Foundation (ESF) under Psik programme, Donostia International Physics Center (DIPC), Ministerio de Educación y Ciencia and National Science Foundation (NSF).

Summary

The School is a shared activity of the three PSI-K working groups, WG1 (GW method), WG2 (quantum Monte Carlo) and WG3 (dynamical mean field theory). It aims at giving a unified overview of the three many-body approaches.

The School is the first Summer School in the Psi-k Marie Curie Series of Events (Psi-k Training in Computational Nanoscience). These Schools are complementary to the Hands-on tutorials offered within the same Programme and aim at providing understanding of the physical phenomena and materials in addition to the computational techniques which are then covered in the hands-on tutorials.

The School is reach out to young researchers already working in the general field of many-body ab-initio theory, as well as researchers who are not yet practitioners but are interested in acquiring the necessary expertise. The School give a solid introduction to the description of electronic correlation effects on an ab-initio basis in both weakly and strongly correlated materials. The activity provided the necessary background and context, highlighting the most challenging problems, and the topics of current interest. Finally, the program achieved a good balance between theoretical and experimental lectures.

For further information, visit the website:

http://www.mc-psi-k-training.cecam.org/index.php?content=activities/tutorial

Description of the scientific content and discussion at the event

Despite the successes of density functional theory (DFT) in describing the electronic structure of complex molecules and solids, the treatment of electronic correlation within a local density approximation (LDA) to DFT is only approximate, often leading to incorrect results for both strongly and moderately correlated systems. An important area of research within electronic structure theory is therefore the development of alternatives to density functional methods. In particular, it is vital for researchers in electronic structure theory to be able to access a hierarchy of techniques that can describe electronic correlations at higher and higher levels of precision.

For the ground and excited properties of real materials in the weak correlation regime, Quantum Monte Carlo (QMC) methods are among the most successful of the post-DFT approaches. The required computing time in QMC scales algebraically as the cube (or better) of the system size, and it has yielded accurate results for the correlated properties of large molecules and solids where conventional quantum chemistry methods are extremely difficult to apply. QMC is establishing itself as a unique tool for exploring electronic correlation in systems of interestto materials science and for obtaining conclusive answers in cases where DFT is shown to be inadequate.

The QMC part of the school will focus on introducing the basics of the method as well as touching on current methodological developments, including efforts to incorporate molecular dynamics and improve geometry optimisation schemes, to find more efficient ways of optimising trial wave functions, and to develop new algorithms alternative to the fixed-node diffusion Monte Carlo method. Speakers involved in pushing the frontier of applications to ever more complex systems such as strongly correlated systems have been also invited.

While structural properties of materials are mainly determined by the static electronic ground state and can be treated within the QMC-scheme for correlated system, the response to external probes in modern non-destructive spectroscopies can only be explained in terms of dynamic excitations. Thus, the knowledge of excited states is essential not only for its fundamental importance in condensed matter physics, but also for the impact in practical applications like the design of new materials with technological or medical interest.

The theoretical foundations of this field are well established, and have been accompanied with physically well-motivated approximations suitable for ab-initio calculations in real materials. Namely, in the context of many-body perturbation theory (MBPT), Hedin's GW approximation has been highly successful in predicting single-particle spectra and quasiparticle lifetimes. It is also used as a first step in the theoretical many-body study of two-particle excitations within the Bethe-Salpeter equation (BSE), which is required to obtain a correct description of photoabsorption spectra. On the other hand, time-dependent density functional theory (TDDFT) is an alternative to calculate optical spectra with neutral excitations, with the important advantage of being more amenable for practical simplifications than MBPT-based schemes.

For strongly correlated systems such as transition metal or rare earth compounds, recent progress has been achieved with the development of a realistic dynamical mean field theory based on the LDA electronic structure (LDA+DMFT). New challenges here related with a basis-independent general implementation of the DMFT scheme based on the first-principle Wannier-function formalism and incorporation of efficient impurity solvers based on continuous-time quantum Monte Carlo approach starting on strong and weak coupling diagramatic expansion. Important development towards the first-principle description of strongly correlated systems connected with unification of the non-local GW approximation and local DMFT technique (GW+DMFT).

Modern electronic structure calculations for materials with strong electronic Coulomb correlations have thus developed into a new research field at the border between band structure theory and quantum many-body problems. Since this area of research requires knowledge of different electronic structure approaches and complicated field theoretical techniques, it is very hard starting problem for young PhD researches. The San-Sebastian summer school have been filled this gap and have allowed the graduate students to acquire simultaneously knowledge and understanding in different parts of the ab-initio many-body theory.

The school have started with the general discussion of the Density Functional Theory (DFT) and its Time Depemdent (TDDFT) generalization.

This lecture have been given by Dr. Robert van Leeuwen from Groningen (The Netherlands) who is the active researcher in this field. Dr. van Leeuwen also discussed the connection of TDDFT scheme to standard many-body Green Function theory. At the same time perfect introduction to new experimental techniques for excitation spectrum of materials have been given by Prof. Franz Himpsel from Wisconsin (USA), who pioneered application of the Angle-Resolved Photoemission Spectroscopy (ARPES) to investigation of real correlated systems. Important basic of so-called GW-scheme in the context of the many body theory for electronic structure was introduced by Prof. Rex Godby from University of York (UK) who is one of the main practitioner of this methods and head of the ESF cluster of excellence. At the end of the fist day, Dr. Miguel Marques from University of Coimbra (Portugal) discussed the application of TDDFT for finite systems, which followed by general discussion on calculation of excited spectrum in molecules and solids by TDDFT scheme.

In the second day Prof. Mikhael Katsnelson from the Radbout University of Nijmegen (The N|etherlands) gave complete introduction to advanced Many-body perturbation theory (MBPT) and general way to calculate excitation spectrum of solid including the spin-wave excitation and optical spectrum. Starting from this many-body background Prof. Steven Louie from University of Berkeley discussed the GW scheme and the Bethe-Salpeter equation to investigate spectroscopic properties of real correlated solids. The first basic lecture on continuum Quantum Monte Carlo methods was given by Prof. Matthew Foulkes from Imperial College London (United Kingdom) who is one of the most active researcher in this field. An important lecture on general introduction to the physics of correlated clectron materials have been presenter by Prof. Dieter Vollhardt from University of Augsburg (Germany) who recently was awarded the Europhysics prize for this research. At the end of the second day an introductory lecture on angle-resolved photoemission spectroscopy (ARPES) and its application to the experimental study of the electronic structure of solids was given by Prof. Andrés Felipe Santander-Syro from Université Paris-Sud (France) followed by short discussion on the many body effects in solids.

The third day was devoted to introduction to Dynamical Mean-Field Theory (DMFT) by Prof. Dieter Vollhardt from University of Augsburg (Germany) who is one of the co-founders of this very important new developments. In the following the diagrammatic (continuous-time) quantum Monte Carlo Methods for classical and quantum spins was introduced by Prof. Matthias Troyer from ETH Zurich (Switzerland) with very interesting presentation of the origin of the so-called sign problem in fermionic QMC simulations. Prof. Ralph Claessen from University of Wuerzburg (Germany) give very useful overview of physics of correlated electron materials from the point of view of experiments with photoelectron spectroscopy. The second lecture on application of Time Dependent Density Functional Theory, in this case to extended systems was presented by Francesco Sottile from Ecole Polytechnique, Paris (France). The applications of Quantum Monte Carlo to Solids have been discussed by Prof. Matthew Foulkes. At the end of this day the prospects and details of the new technique for electronic structure calculation of correlated solids, so-called LDA+DMFT scheme was given by Prof. Silke Biermann Ecole Polytechnique, Paris (France) following be general discussion on the problem of first-principle calculations of effective electron-electron interactions in solids.

The third day was devoted to realistic QMC scheme and Prof. Lubos Mitas from North Carolina State University, (USA) gave the impressive example of practical implementation of Quantum Monte Carlo for nanosystems and materials resulting in accurate description of electronic structure and dynamics. In addition, a novel so-called Resonating Valence Bond (RVB) approach for QMC simulations was discussed by Prof. Sandro Sorella from SISSA, Trieste (Italy). The correlated effects in f-electron materials within the Self-Interaction Correction (SIC) Scheme have been introduce by Dr. Dzidka Szotek from Daresbury (United Kingdom). The second part of diagrammatic continuous-time quantum Monte Carlo Methods for fermions was given by Prof. Matthias Troyer. An important new development of Wannier functions in the context of the Dynamical Mean-Field Approach to strongly correlated materials presented by Prof. Frank Lechermann from University of Hamburg (Germany). An interesting cluster generalization of the DMFT methods was introduced by Dr. Olivier Parcollet from CEA-Saclay (France).

The last day of the school start from the discussion on topology of fermion nodes and pfaffian wavefunctions by Prof. Lubos Mitas. A new important development to go beyond simple DMFT approximention within so-called Dual-fermion Approach to Nonlocal Correlations was introduce by Prof. Aleksey Rubtsov from Moscow State University. And finally Prof. Liu Hao Tjeng from University of Cologne (Germany) presented the crucial experimental talk on the testing modern theories for correlated systems. The school was ended with general panel discussion on perspectives and practical importance of the new development in the field of correlated electron materials.

Assessment of the results and impact of the event on the future direction of the field

The School on Ab-initio Many-Body Theory in San-Sebastian was very well presented by young researchers all over the Europe and considered to be a successful attempt to introduce a comprehensive scheme for practical investigation of correlation effects in electronic structure calculation of real materials. The students and postdocs from different fields of computational materials science and many-body scheme were discussed futures of the Ab-initio Many-Body Theory for real materials. The number of applications (above 250) surpassed all expectatives and, of course, the limit of 90 places that we had to satisfy in order for the students to get the maximum benefit from the school, and also due to space and computer resource limitations. The students (graduate and postgraduate) also did actively participate in the round-tables and discussions.

The impact of this school on the future direction of correlated electronic structure is clearly seen on the very active discussion on the final panel meeting concerning the predictive power of new many-body scheme for realistic materials. It is clear that all participants will be involved in the future in the developments on accurate scheme for complex structure of correlated materials and nanosystems. The important future development in the field will be related with unifications of efficient LDA+DMFT scheme with accurate GW or TDDFT methods in electronic structure calculations, which was discussed in the present summer School in San-Sebastian.

Final programme of the meeting

All lectures can be found on the website:
http://dipc.ehu.es/arubio/mbschool.php

MONDAY, JULY 23rd

8:45 h Registration

9:00-10.30 Introduction to density functional theory (DFT) and time-dependent DFT
Dr. **ROBERT VAN LEEUWEN**
Rijksuniversiteit Groningen, The Netherlands

10:30-11.30 New experimental techniques for excitation spectrum of materials
Prof**.** **FRANZ HIMPSEL**
University of Wisconsin, USA

Coffee Break

12.00-13.30 Many-body theory in a nutshell and Hedin equation (GW)
Prof. **REX GODBY**
Univertity of York, United Kingdom

Lunch

16.00-17.30 Theoretical advances in time-dependent DFT
Dr. **ROBERT VAN LEEUWEN**
Rijksuniversiteit Groningen, The Netherlands

17.30-18.30 Aplications of TDDFT to finite systems
Dr. **MIGUEL MARQUES**
University of Coimbra, Portugal

18:30 Discussion session: TDFT and excitation spectrum of materials

TUESDAY, JULY 24th

9:00-10.00 Advanced Many-body perturbation theory (MBPT)
Prof **. MIKHAIL KATSNELSON**
Radboud University of Nijmegen, The Netherlands

10.00-11.30 GW and Bethe-Salpeter Equation Approach to Spectroscopic Properties
Prof **. STEVEN G. LOUIE**
University of California at Berkeley, United States

Coffe Break

12:00-13.30 Introduction to continuum quantum Monte Carlo (QMC) methods
Prof **. MATTHEW FOULKES**
Imperial College London, United Kingdom

Lunch

16.00-17.00 Introduction to the physics of correlated materials
Prof. **DIETER VOLLHARDT**
University of Augsburg, Germany

17.00-18.00 Experimental techniques for correlated materials
Prof. **ANDRÉS SANTANDER-SYRO**
Université Paris-Sud, France

18.00 Round table: Basics of ab-initio and MBPT techniques

WEDNESDAY, JULY 25th

9.00-10.00 Introduction to dynamical mean field theory (DMFT)
Prof **. DIETER VOLLHARDT**
University of Augsburg, Germany

10.00-11.00 Introduction to Quantum impurity solvers
Prof **. MATHIAS TROYER**
ETH Zurich, Switzerland

Coffee Break

11:30-12.30 Physics of correlated materials: Experiments
Prof **. RALPH CLAESSEN**
University of Wuerzburg, Germany

12.30-13.30 Applications of TDDFT to complex systems
Dr. **FRANCESCO SOTTILE**
Ecole Polytechnique, Paris, France

Lunch

16.00-17.00 Applications of quantum Monte Carlo to solids
Prof **. MATTHEW FOULKES**
Imperial College London, United Kingdom

17.00-18.30 Prospects of LDA+DMFT calculations
Prof **. SILKE BIERMANN**
Ecole Polytechique Paris, France

18.30 Discussion session and Round table: Correlated materials and LDA+DMFT

THURSDAY, JULY 26th

9.0.10.0 Quantum Monte Carlo for nanosystems and materials: Electronic structure and Dynamics.
Prof **. LUBOS MITAS**
North Carolina State University, United States

10.0-11.00 A novel resonating valence bond approach for QMC simulations
Prof **. SANDRO SORELLA**

SISSA, Trieste, Italy

Coffee Break

11:30.12.30 Self interaction correction (SIC) scheme and f-electrons materials
Dr. **DZIDKA ZSOTEK**
Daresbury, United Kingdom

12:30-13.30 Continuous time Quantum Monte Carlo method
Prof. **MATHIAS TROYER**
ETH Zurich, Switzerland

Lunch

16.00-17.00 General DMFT scheme in Wannier basis
Prof. **FRANK LECHERMANN**
University of Hamburg, Germany

17:00-18.30 Cluster extension of DMFT scheme
Dr. **OLIVIER PARCOLLET**
CEA-Saclay, France

18:30 Discussion session and Round table: Applications of DMFT and QMC

FRIDAY, JULY 27th

9:00-10.15 QMC: the fixed-node problem and the topology of fermion nodes
Prof**. LUBOS MITAS**
North Carolina State University, United States

10:15-11.15 Beyond DMFT: dual fermion approach for non-local correlations
Prof. **ALEKSEY RUBTSOV**
Moscow State University, Russia

Coffee Break

12:00-13:00 Testing modern theories for correlated systems
Prof. **LIU HAO TJENG**
University of Cologne, Germany

Lunch

16:00-18:00 Synthesis session, Concluding remarks and Round table: frontiers in the field new challenges