

1) TITLE:

Ab Initio Spectroscopy of Electronic Excitations: a decade of applications of the Bethe-Salpeter Equation.

Louvain la Neuve, September 13.-16. 2006

PURPOSE:

The aim of this four-day workshop is to assess the present status, the latest achievements and future perspectives of first principles approaches to the study of spectroscopic properties of solids, nanostructures, systems with increasing complexity, and materials of technological and biological interest. More specifically, this workshop will offer the opportunity to take a look back on ten years of developments and applications of the Bethe-Salpeter Equation method for the accurate calculation of optical and dielectric spectra. Open questions, achievements, advantages, and drawbacks of the Bethe-Salpeter Equation will be contrasted with other approaches in order to stimulate discussions about the future of the field and to bring together scientists from different communities where electronic excitations are calculated.

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2. SCIENTIFIC CONTENT AND MOTIVATION

While structural properties of materials are mainly determined by their static electronic ground state, the response to external probes in modern spectroscopies can often only be explained in terms of dynamic excitations. A thorough understanding of excited state properties is therefore essential not only for their fundamental importance in Condensed Matter Physics and in Nanosciences, but also for their role in practical applications like the design of new materials with technological or biological interest. The theoretical foundations of this field are well established, and have been accompanied by physically well-motivated approximations suitable for ab-initio calculations in real materials. E.g., for the prediction of single-particle spectra and quasiparticle lifetimes many-body-perturbation-theory (MBPT) in Hedin's GW approximation [1] has been highly successful [2]. The GW method is also used as a first step in an ab initio many-body approach to two-particle excitations through the solution of the Bethe-Salpeter Equation (BSE), which allows to obtain a correct description of photoabsorption spectra [3,4]. On the other hand, time-dependent density functional theory (TDDFT)[5] provides an alternative to calculate optical spectra. TDDFT has the important advantage of being computationally more efficient and also more amenable to practical simplifications than MBPT-based schemes [4]. The disadvantage of TDDFT is, of course, the uncertainty of accuracy due to the unknown time-dependent exchange-correlation functional. Both the BSE and the TDDFT approach have been applied to a wide variety of systems, ranging from simple atoms to systems with prospective technological interest. Combined, they provide a reliable interpretation of experiments such as photoemission, photoabsorption, electron-energy-loss spectroscopy, X-ray absorption or scanning-tunneling microscopy [2,4]. Until now, these excited states methods have been mostly applied assuming stationary nuclei. The extension to excited states nuclear dynamics is an important current development.

The proposed workshop is intended to provide a forum to discuss the advances in the theoretical and computational treatment of optical and dielectric spectroscopy. The focus will be on the Bethe-Salpeter Equation method of MBPT. In the last ten years, it has emerged as the most reliable

approach for describing neutral excitations. These years have also seen the development of sophisticated efficient numerical algorithms and codes for the solution of the BSE, and, as a consequence, an increasing number of applications in different fields. In the BSE approach, the calculation of response functions requires the solution of a 2-particle equation which explicitly contains the dynamics of electron-hole pairs, created through absorption of a photon, in the form of appropriate Feynman diagrams. The electron-hole interaction can lead to bound states within the gap and/or to strong spectral deformations above the continuum absorption edge. The BSE allows for an accurate description of these excitonic effects. However, the explicit diagrammatic approach makes the method numerically expensive and effectively restricts its application.

Recently, new developments within TDDFT have opened up an alternative route for the accurate calculation of optical spectra including excitonic effects: the design of exchange-correlation kernels in close comparison with the concepts of many-body perturbation theory. In TDDFT the time dependent density replaces the static density of DFT as the fundamental variable, which makes TDDFT computationally much more efficient than the Green's function based BSE scheme and thus potentially more suitable for applications to large and complex systems. An inherent drawback of TDDFT is, however, that it does not presently allow for an immediate interpretation of the results in terms of neutral excitation energies and excitonic wavefunctions as this is the case in the BSE approach, even though excitonic effects are correctly accounted for in the final observable spectra. It is important to note in this context that most of the recent progress on TDDFT has resulted from a comparison with BSE.

The purpose of the proposed workshop is to bring together experts and researchers from different fields to review the developments and achievements of the last ten years of BSE.

Topics to be covered:

- History and recent developments of BSE
- Ab-initio implementations of BSE
- Semi-empirical implementations of BSE (e.g., in a tight-binding framework)
- Application of BSE to new systems and new materials (e.g., nanoclusters, nanowires, nanotubes, bio-molecules)
- New implementations and higher order contributions (e.g., vertex corrections)
- advantages and disadvantages of BSE
- comparison with TDDFT
- comparison with configuration-interaction methods in quantum chemistry
- Recent advances in spectroscopy
- Other recent developments in electronic structure theory

The motivation for the organization of the workshop is:

- i) to offer the possibility for discussions between researchers with different experiences and points of view,
- ii) to assess the latest achievements and the perspectives of these theoretical approaches (both BSE and TDDFT BSE-derived), to discuss their drawbacks and their advantages;
- iii) to attract young researchers to this developing field in order to increase the number of scientists involved in activities of this kind, and to foster links between different research groups working on electronic excitations from first-principles.

To realize these objectives we propose a meeting with a broad scope.

It is our aim to stimulate the scientific discourse between scientists from different communities and to promote the application of ab-initio methods to systems with immediate interest beyond those of fundamental research. With regards to the latter input from experimental groups is highly important.

The progress in the theoretical treatment of electronic excitations and spectroscopy is reflected in the continuing series of workshops devoted to this topic and in the increasing number of participants. The proposed meeting follows previous workshops on 'Excited Electrons in Molecules, Solids and Atoms' (Lyon,1997), 'Spectroscopy of Electronic Excitations in Materials' (Valladolid,1998), 'Calculation of Electronic Excitations in Finite and Infinite Systems' (Lyon, 1999) 'Excited States and Electronic Spectra' (Lyon,2000), 'Ab-initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials' (Lyon, 2002), 'Ab-Initio Electron-Excitations Theory: Towards Systems of Biological Interest' (San Sebastian 2003), 'Theory and Modelling of Electronic Excitations in Nanoscience', (Maratea 2004), and '40 Years of the GW Approximation for the Electronic Self-Energy: Achievements and Challenges', (Bad Honnef 2005).

These workshops have had an acknowledged contribution to the establishment of a very strong community of scientists interested on applications of MBPT and/or TDDFT in Condensed-Matter Physics. Hence we propose to continue this series with a cycle of 4 new workshops, the first in Belgium, then in the Rhone-Alpes french region, the third in Sicily and the last probably again in Rhone-Alpes. As described, the meeting in 2006 will have a broader scope, but we would like to keep the overall format of preceding conferences: an informal, general style, ample time devoted to discussions and round-tables, and preference given to contributions by young scientist. Since the main goal of this workshop is to explore future applications and prospects for ab-initio techniques, we are confident that a friendly atmosphere will be more conducive to the achievement of this objective.

References:

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E.K.U. Gross and W. Kohn,

3. INVITED SPEAKERS:

We primarily intend to invite scientists whose expertise lies in state of the art many-body and BSE theory and also in time-dependent DFT. However, there will be a considerable number of invited speakers who are acknowledged experts in other areas of theoretical physics related to excited states or whose area of expertise are spectroscopical techniques that are currently used to characterize excited-state properties experimentally.

TENTATIVE LIST:

Hanke or Strinati or both (BSE review)
E.K.U. Gross (Germany) (review TDDFT)
L. Reining (France) (ab initio BSE pioneer + LRC- MT-TDDFT)
S. G. Louie (Berkeley, USA) (ab initio BSE pioneer) (possible replacement Tiago: BSE polyacetylene poliacene)
E. Shirley (NIST USA) (ab initio BSE pioneer)
R. Del Sole (Italy) (ab initio BSE pioneer + f_{xc} kernel MB1WPT)
Stubner or Tokatly or Pankratov (TDDFT theory develop.)
M. Bonitz (real-time Kadanoff-Baym, T-Matrix, excitons, biexcitons and trions)
G. Schmidt (Universitat Jena, Germany) (BSE $O(N^4)$ efficient method)
Koinov (BSE and Magnetoexcitons)
Hummer or Ambrosch-Draxl (BSE in organic molecular crystals)
Neng-Ping Wang or (Rohlfing) (BSE on CO adsorbate on MgO or other insulator surfaces)
E. Chang or E. Molinari (BSE on Nanotubes)
G. Cappellini (BSE applications)
G. Allan (tight-binding methods for optical spectra of complex systems)
C.O. Almbladh (Green's function methods)

4. PARTICIPANTS

The call for participation will be mainly directed at scientists specialized in theoretical and computational physics. Contributions ranging from fundamental studies to semi-empirical approaches for complex phenomena are encouraged. The target number lies at approx. 90 participants. In order to ensure maximum interaction between scientist coming from different communities, active participation in the round-table sessions is encouraged. In addition plenty of time for questions and discussions after each oral presentations will be reserved in the scientific program.

Attendance of graduate students and postdocs will be strongly encouraged through the inclusion of short contributed talks and poster sessions with brief oral introductions. Furthermore, we will encourage Ph.D. students who presented an outstanding poster to convert it into a short talk. We feel that the inclusion of young researchers is a very important point, because as the "scientists of tomorrow" they are the basis of a strong and healthy scientific community.

5. FORMAT

The format of the workshop will be similar to the previous workshops listed in section 2, since this has been proven the best way to stimulate discussions between participants and provide an informal environment. Each conference day will be divided into a morning session (9:00--12:40) and an afternoon session (15:30--20:00), both with coffee-break intervals. Invited talks will be allocated up to 40 minutes plus 20 minutes reserved for discussion. In addition, up to 90 minutes will be

reserved for one round-table discussion. Poster sessions, chaired by an invited speaker, will be preceded by short oral introductions.

6. TUTORIAL ELEMENTS AND ATTRACTION OF NEW RESEARCHERS

To further emphasize the training aspect of the workshop in particular for newcomers to the field two experienced scientists (e.g. L. Reining and E.K.U. Gross) will be invited to give a review seminar on the state of the art of Bethe-Salpeter and TDDFT-based applications. These review seminars are intended to be tutorials for those interested in BSE or TDDFT, but without previous experience in either of the two methods or with ab-initio calculations in general. The sessions will provide more time for scientific discussions and will give, in particular the young researchers, the opportunity to present their work and to get in contact with fellow scientists and senior researchers. Since the objective of the proposed workshop is to stimulate scientific discourse by means of oral presentations and poster sessions, we do not plan to hold specific tutorials on excited-state calculations. Nonetheless, ample break time between sessions will give all students and postdocs the opportunity to share their current research with senior scientists. Finally, the research group leaders will be invited to advertise job and fellowship opportunities as well as other relevant conferences on their respective fields of interest.

7. FINANCIAL INFORMATION

We estimate a total cost of 50.000 euro for the conference. This amount includes all the expenses for inviting speakers, scholarships for selected young scientists, and additional costs for stationery, publicity, coffee breaks, or abstract books. The Université Catholique de Louvain will provide one of its main conference rooms and all the necessary equipment, so the related expenses are not included in the above estimation. We aim to encourage the participation of young researchers. For this reason we allocate all funding from the Psi_k Network to the financial support for PhD students or postdocs. (The minimal condition for receiving a scholarship will be an active contribution in form of a talk or a poster presentation.) We hope to offer grants totalling 550 Euro: 290 Euro living allowance, plus 260 Euro for travel expenses. Therefore we apply for a total amount of 15.000 Euro.

8. CO-SPONSORSHIP

We will apply also to local institutions (FNRS-Belgium and the Université Catholique de Louvain) to get funds for invited speakers. Thanks to the co-organization with an American scientist (Prof. John Rehr) we will ask some funding from U.S.A. institutions (DOE, NSF) to sponsor the participation of American researchers.

9. LOCATION

The workshop will take place on 13-16 September 2006 in Louvain-la-Neuve (Belgium). The Université Catholique de Louvain has longstanding experience in hosting conferences and scientific meetings and will provide an excellent framework for fruitful scientific exchange between the participants in an informal atmosphere.

10. CONTACT TO AMERICA - CO-ORGANISATION

Prof. J. R. Rehr at the University of Washington, coordinator of the FEFF Project (<http://leonardo.phys.washington.edu/feff>) and the CSMN Project (<http://www.phys.washington.edu/~cmsn/CRTs/EESRF>) has accepted to be co-organizer of the conference.

We believe that this initiative will boost also the collaboration with researchers in the USA, who work at the forefront of nanoscience, and exchange expertise and knowledge between Europe and USA.