Workshop Scientific Report (ESF)

Workshop: Perspectives and challenges of many- particle methods: efficient strategies and tools for describing complex systems

Organizers: Prof. Dr. Thomas Frauenheim, University Bremen, BCCMS, Germany
Prof. Dr. Alexander Lichtenstein, University of Hamburg, Germany
Prof. Dr. Christian Ochsenfeld, Technical University Munich, Germany
Prof. Dr. Andreas Savin, University Pierre Marie Curie, Paris, France

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I. Summary

The workshop "Perspectives and challenges of many- particle methods: efficient strategies and tools for describing complex systems" was held at the University of Bremen, Germany from September 19th to 23rd 2011. In total, 78 participants from Austria, China; France, Germany, Israel, Italy, The Netherlands, Norway, Russia, Spain, USA, UK, Denmark, Japan, Sweden, Switzerland attended the workshop.

The programme consisted of 30 invited lectures, one poster session presenting 32 posters and many events (reception / conference dinner) to allow for informal exchange. The lectures were scheduled to last 40 min, including 5-10 min discussion time. In addition to this extended time for discussion, the chairpersons were instructed to introduce the subject of the session and to actively participate in the discussion. This "Gordon-conference-style" was essential to guarantee a vivid discussion. The organizers ensured that well-established scientists acted as invited speakers and chairpersons.

Concerning the poster session, we accepted only 32 posters to allow for an intense exchange of ideas at each single poster. Here, we encouraged in particular the young scientists to ask questions. The participation of PhD students was supported by partly covering local accommodation costs.

Due to the compact organization and accommodation in one hotel only all participants had to stay together for the whole time of the conference, which additionally enforced the scientific discussion which was mandatory since scientists from various separated fields, i.e. advanced quantum chemistry, quantum Monte-Carlo, many-body perturbation theory, time-dependent DFT, etc. were attending the meeting to merge ideas and formulate a common goal for future method developments.

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II. Scientific content and discussion

The field of computational material science made recently a tremendous step toward a first-principle description of correlated electronic systems including transition metal and rare-earth elements. A great impact is expected in the new area of artificially constructed magnetic nano-systems and at the interface of traditional inorganic chemistry, physics, biology and materials science in general. Of prime importance is the development of next-generation realistic many-body computational tools which are fast, reliable and are able to describe non-trivial quantum dynamics of complex systems. In order to address these problems, new integrated software tools for realistic quantum simulations of correlated systems need to be developed for a broad scientific community.

Recently a new generation of continuous-time Quantum Monte Carlo (CT-QMC) methods for numerically exact calculation of complicated fermionic path integrals have been proposed for interacting electrons based on the weak-coupling and strong-coupling perturbation expansion. This methodological breakthrough in the quantum many-body theory stimulate a great progress in the electronic calculations of realistic and increasingly complex strongly correlated systems within the dynamical mean-field theory (DMFT) where the solution of effective multiband impurity problem is the main point. New QMC technique stimulate the fast and important developments in the field of strongly correlated materials related with the realistic LDA+DMFT calculations for the d- and f-orbital cases, heavy-fermion systems, strongly correlated thermoelectric compounds and novel high-temperature superconducting pnictides.

Over the past decades, density functional theory (DFT) has become the effective single-particle theory of choice both for physicists from the solid state community as well as for quantum chemists. However, this tremendous success is also accompanied by an ever growing list of documented failures, especially for strongly correlated systems. Modern approaches to improve the description by better exchange-correlation functionals are based on an adapted treatment for short and long-range electron-electron interaction (so called range-seperated functionals) or the seperate treatment of exchange and correlation functionals (exact exchange + random phase approximation).

Beyond DFT, the GW/BSE approximations based on MBPT have found widespread use in the calculation of single-particle spectra. Originally used only to compute band structures in solids, GW has recently also been applied to study surfaces and molecules. A detailed comparison of the self energy in the GW context with the exchange-correlation functional in DFT, is expected to pave the road for further improvement of functionals. This interplay of different approaches to correlated systems was already exploited in the realm of time dependent DFT.

Yet other approaches for interacting many-electron systems were put forward in the quantum chemistry community. Wavefunction-based schemes allow to systematically approach the exact solution of the electronic Schroedinger equation and in this way offer a hierarchy useful for estimating error bars of simpler approximations. The methods range from efficient MBPT methods mostly employing Gauss-type basis functions to coupled-cluster theory and also multi-reference approaches. To deal with the cusp problem and basis deficiencies, r12 and more recently F12 methods have been brought forward. The steep increase of the computational effort with molecular size has been circumvented by introducing linear-scaling methods for many quantum-chemical methods and for computing various molecular properties. They

exploit the local electronic structure and open the way to treat large molecular systems with 1000 atoms and more at the HF, DFT, and MP2 levels. Also the possibilities in performing highly accurate CC calculations has been dramatically increased. Finally, also partially periodic boundary conditions have been accounted for. The relation of all of these schemes to the correlated methods in the many-body physics community is just now starting to be on a systematic level.

An interesting first-principle alternative to LDA+U scheme for correlated materials is related with developments of Reduced-density-matrix-functional theory (RDMFT). It is based on old Gilbert's theorem, which shows that the expectation value of any observable in the ground state can be expressed as a functional of the one-body reduced density matrix. The advantage of RDMFT approach, compared to DFT, is that the exact many-body kinetic energy is easily expressed in terms of reduced-density-matrix. The RDMFT calculations of transition metal oxides gives correct insulating states of these correlated compounds.

The variety of approaches show the zoo of methods to tackle the highly complex many-body problem. Although there are many links between the methods, it is often highly difficult to find unifying features. The very lively discussions in the workshop clear showed the different languages, but also the many common features in aiming for the ultimate goal of solving the many body problem, which made the workshop a full success.

While density-functional being in principle exact, the lectures clearly showed the many difficulties in developing better functionals and to step up Perdew's advocated Jacob's ladder.

Another central problem clearly appearing in several talks is not only the treatment of dynamic correlation, but also of static correlation. While many attempts have been and are made, the path towards cost-efficient and highly accurate schemes is still a major challenge. A brute force scheme often used as a reference is certainly QMC, however, the difficulty of a statistical method and the systematic error control at realistic costs is clear. In particular the lack of error cancellation in relative energies remains a drawback. Nevertheless, the importance of reliable benchmarks is always present and here QMC and CC methods are central to calibrate and understand simpler approximations to the many-body problem. The developments made in these areas presented in several lectures are highly impressive.

Also the field of basis expansions remains a challenge: in plane-wave codes the use of ECP remains an issue, while in Gaussian-type basis sets the influence of basis deficiencies and basis-set superposition errors (both inter- and intra-molecular BSSE) plays a major role. For the latter so-called F12 methods for describing the cusp have shown major improvements

During the workshop there were many important discussions on the challenges and future directions of realistic many-body methods for electronic structure calculations. After the talk of Prof. S. Louie on GW-approach the ultimate limit for the size of simulation system in the present GW-program and in the future approach have been discussed. The question of possibility to investigate the dipole-forbidden d-d transitions in optical spectrum of NiO within the Bethe-Salpeter (BS) equation was discussed after the talk by Prof. F. Bechstedt. It was pointed out that the first-principle investigations of optical spectra for strongly correlated oxides will be possible in the near future. Possible collaborations with the DMFT-community on the problem of vertex-corrections in optical spectrum of correlated oxides will be very useful for the GW-community.

The talk by Prof. S. Biermann on the DMFT extension to GW –scheme have been generated a discussion on the progress of QMC calculations with screened Coulomb interactions. It was pointed out that if numerically exact solution of the local quantum impurity problem with frequency dependent interactions is possible for multiorbital d- and f- systems, then one can efficiently combined the GW+DMFT scheme to treat correlation effects in transition metal and rare-earth materials. In this case the new possibilities is open in the research on new class of Fe-based high-temperature superconductors, were both non-local spin-fluctuation effects and local Coulomb correlations are important for understanding the mechanism of non-convention electron pairing phenomena.

During the session on DFT+DMFT (Profs. V. Rubtsov, K. Held and M.R. Valenti) an important question on the accuracy of continuous-time QMC scheme for realistic heterostructure and cluster calculations have been discussed. Different aspects of the interaction- and hybridization-expansion CT-QMC methods for multiorbital correlated impurity problems was analyzed. The development of the optimal CT-QMC solver will be an important task for the DMFT-community in future.

A discussion on the future of many-body perturbation scheme for a finite quantum systems, after the talk by Prof. M. Scheffler, was very useful for future of GW, CC and other methods. Moreover, the similar discussion (Prof. G. Kresse) on the quality of self-consistent GW scheme which include not only the direct, but also the exchange second-order, in the screened Coulomb potential, contribution to the total energy, shows a very good agreement with an accurate CC-results. This can be of crucial importance for the future approach to the many-body perturbation scheme for realistic correlated systems and also shows an creative collaboration between physics and quantum-chemistry communities.

III. Assessment of the results and impact on future direction of the field

With its focus on many-body methods, the workshop brought together researchers from a wide variety of different backgrounds and very different 'scientific languages'. Although there are many common features, the complexity of the methods makes it often very difficult to find more useful links and in this way to approach better solutions to the many-body problem which is of central importance. Therefore many more meetings of this kind are highly desirable and can help to find better approaches that allow to describe materials - and complex systems in general - in a much more accurate and efficient way. Therefore, a follow-up workshopsevery two or three years would be desirable.

The objectives of the workshop have been fully achieved. The workshop became a forum to brainstorm ideas about solutions to important correlated-electrons problems and identify new directions for many-body method development and challenging applications. There is ongoing intensive exchange of benchmark data between the many-body physics and the correlated quantum chemistry community while both communities are approaching applications to more complex and larger realistic systems.

The most advanced computational methods nowadays achieve a predictive level close to experimental data of materials properties and functions. In analysing this, there is a paradigm change. Computational applications are not anymore aiming only at interpreting experimental results but rather predict new materials systems and devices. The delivery of this new computational technology to a broad community in future will facilitate breakthroughs on high-impact materials science problems in nano-science, biophysics and new energy storage.

There are lots of ongoing discussions between the different development directions (QMC, MBPT in quantum chemistry and physics, development of new functional, etc.), (though competition) even close intense collaborations for validating the methods against each other and pushing the field to the limits of quantitative accuracy.

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The Organizers