Report for the workshop

Fundamental Challenges of Electron-Density-Based Approaches to Time-Dependent Processes and Open Quantum Systems (ElDeBaAp)

Date: June 24th-26th 2019
Location: ETH Zürich, Switzerland
Website: https://eldebaap-workshop.ethz.ch
Organizers: Axel Schild (ETH Zürich), Jakub Kocák (ETH Zürich)

From 24th to 26th June 2019 the workshop "*Fundamental Challenges of Electron-Density-Based Approaches to Time-Dependent Processes and Open Quantum Systems*" (ElDeBaAp) took place at ETH Zürich, Switzerland. This workshop gathered experts on DFT, TDDFT, density cumulant theory, Green's function approaches and density matrix methods to discuss theoretical challenges of their approaches and open problems that have to be solved.

Motivation:

Effective single- or few-electron methods based on the electron density or density matrix are often the methods of choice for the calculation of the electronic structure and properties of molecular systems. Some of them are well-developed and can be used to obtain a reasonably accurate result also for larger systems.

In recent years there has been interest in making these methods more accurate and in applying or extending variants of these methods to open quantum systems and to time-dependent phenomena. While a quantum-mechanical description of the electronic properties alone is already a formidable task, making the electronic system an open quantum system by inclusion of effects such as nuclear motion, time-dependent external interactions, or coupling to other degrees of freedom that are not explicitly treated, poses new challenges that want to be overcome.

The workshop gathers developers of a variety of electron density-related approaches together to name and discuss these problems. Emphasis is placed on the theoretical challenges and on comparing the advantages and limitations of the selected methods. Next to scientists working on open systems, also some experts working on selected aspects of the theory of closed systems are invited to broaden the range of ideas.

Participants:

- Hilke Bahmann (Universität Potsdam, Germany)
- Joachim Burgdörfer (TU Wien, Austria)
- Kati Finzel (TU Dresden, Germany)
- E.K.U. Gross (MPI Halle, Germany)
- Jakub Kocák (ETH Zürich, Switzerland)
- Eli Kraisler (The Hebrew University Jerusalem, Israel)
- Stefan Kurth (Ikerbasque San Sebastián, Spain)
- Lionel Lacombe (City University New York, USA)
- Neepa T. Maitra (City University New York, USA)
- Margherita Marsili (University of Padova, Italy)
- Ryan Requist (MPI of Microstructure Physics Halle, Germany)
- Pina Romaniello (Université Paul Sabatier, France)
- Costanza Ronchi (Universita' di Milano-Bicocca Milano, Italy)
- Rajarshi Sinha-Roy (CEMES/CNRS Toulouse, France)
- Axel Schild (ETH Zürich, Switzerland)
- Alexander Yu. Sokolov (The Ohio State University, USA)
- Mary-Leena Tchenkoue (MPI for the Structure and Dynamics of Matter Hamburg, Germany)
- Iris Theophilou (MPI for the Structure and Dynamics of Matter Hamburg, Germany)
- Carsten A. Ullrich (University of Missouri, USA)
- Vittoria Urso (Università del Salento, Italy)

Program

June 24th	Talk	Topic
09:30-10:00	Registration	
10:00-10:15	Welcome	
10:15-11:15	**Gross**	Laser-induced spin dynamics - predictions from TDDFT
11:15-11:50	Break	
11:50-12:50	**Ullrich**	(TD)DFT for noncollinear magnetism: approximations versus exact benchmarks
12:50-14:15	Lunch	
14:15-15:15	**Burgdörfer**	Solid-state high harmonics : TDDFT and decoherence
15:15-16:15	**Maitra**	Memory in TDDFT: Exact Features and Approximations
16:15-16:50	Break	
16:50-17:50	**Kurth**	Steady-State Density Functional Theory: from Differential Conductances to Many-Body Spectral Functions
18:00-20:00	Posters	

June 25th	Talk	Topic
09:15-10:15	**Romaniello**	Correlation and spectroscopy in many-body theories
10:15-11:15	**Theophilou**	Kinetic energy Density Functional Theory
11:15-11:50	Break	
11:50-12:50	**Schild**	Exact Factorization Approach to the Dynamics of Molecules in Strong Laser Fields
12:50-14:15	Lunch	
14:15-15:15	**Sokolov**	Linear-response density cumulant theory for excited electronic states
15:15-16:16	Discussion	
19:00-22:00	Dinner	

June 26th	Talk	Topic
09:15-10:15	**Kraisler**	Two properties of the exact Kohn-Sham potential and the relationship between them
10:15-11:15	**Finzel**	Orbital-free density-functional theory -- new approaches to old ideas
11:15-11:50	Break	
11:50-12:50	**Bahmann**	From global to local - hybrid density functionals for weak and strong correlation
12:50-14:15	Lunch	
14:15-15:15	**Requist**	Density functional theory of electrons and nuclei based on the exact factorization method: Overview and open problems
15:15-15:21	Closing	

Presented Posters

- Costanza Ronchi:
  Unravelling dynamical and light effects on functionalized titanium dioxide nanoparticles for bioconjugation
- Rajarshi Sinha-Roy:
  Identifying Electronic Modes in Metal Clusters from Delta-kick Calculations
- Margherita Marsili:
  Real time electronic dynamics of molecules close to a plasmonic nanoparticle: combining GW-BSE, Stochastic Schroedinger equation and PCM approaches
- Lionel Lacombe:
  Electronic Embedding via Exact Factorization
- Mary-Leena Tchenkoue:
  Exchange correlation potential in time-dependent current density functional theory
- Vittoria Urso:
  Investigation of kinetic functionals applied to metal nanoparticles.

Discussion session

On Tuesday afternoon, there has been a discussion session regarding the challenges that density-based approaches currently face when being applied to time-independent and time-dependent problems as well as to open quantum systems. The discussion focused mainly on Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT).

One aspect that was discussed is the limited understanding of properties of the exact Kohn-Sham (KS) potentials appearing in DFT. In this respect, the problem of electronic decoherence was mentioned. Is was discussed if dynamical steps appearing in the KS potential are relevant and to what extend decoherence is basis-set dependent. It was also asked how scattering can be described in a DFT framework. Finally, strongly correlated systems were mentioned as a major challenge for DFT, in particular in the context of stretched molecules or molecular dissociation, but also with respect to solid-state systems. As an interesting problem in this respect, a chain of hydrogen atoms was mentioned: KS-DFT predicts that this system is a metal, although it is an insulator. Possible solutions to this problem were discussed.