MM 37: Development of Calculation Methods I

Time: Thursday 15:45–17:00 Location: SCH/A315

MM 37.1 Thu 15:45 SCH/A315

The two-particle Green's function in the particle-particle channel: A survey of approximations — •Caja Annweiler[1], Lucia Reining[2], and Claudia Draxl[1] — [1]Humboldt Universität Berlin, Berlin, Germany — [2]École Polytechnique, Palaiseau, France

While in general setting up and solving the Bethe-Salpeter equation (BSE) is out of reach for realistic systems, it provides an ideal starting point for constructing approximations. In the particle-hole channel, this has lead to established approaches such as the *GW*-level approximation to capture excitonic effects. This framework can be extended to the BSE in the particle-particle channel (pp-BSE), obtained by choosing a different time-ordering in the two-particle Green's function. The result is an equation describing the propagation of two particles (either electrons or holes). While formally similar to the ph-BSE, it is a promising alternative for the calculation of the exchange-correlation energy and yields important information for topics such as pair correlations in superconductors. Despite growing interest in the pp-BSE, systematic investigations of approximations remain scarce.

In the present work we consider a variety of approximations to the pp-BSE. For this purpose, exactly solvable model systems of interacting electrons provide valuable insights into the minimal ingredients needed to capture the key physics. We present approximations from many-body perturbation theory (HF, GW, etc.) at the level of the self-energy Σ and interaction vertex Ξ on small Hubbard models, with the aim of advancing our understanding of approximations in the pp-channel.

MM 37.2 Thu 16:00 SCH/A315

Reliable Super-Resolution for Real-Time Electronic Structure Theory — •Alexander Gorfer, Karsten Reuter, and Matthias Kick — Fritz-Haber-Institut der MPG, Berlin

Calculating excited state spectra of large systems is often prohibitively expensive with standard frequency-domain methods such as the Casida equations, the Bethe-Salpeter Equation (BSE), or Equation-of-Motion Coupled Cluster (EOM-CC). Real-time methods provide an alternative, as all modes are excited simultaneously. However, long simulation times are required to resolve narrow spectral features with traditional Fourier signal analysis, significantly limiting system size. Super-resolution methods such as Compressed Sensing promise high-resolution spectra from much shorter signals but assume the spectrum to be sparse, an assumption which breaks down in larger systems where sharp features are embedded in a quasi-continuum of smaller nearby peaks. To overcome this, we combine newly designed highly noise-tolerant super-resolution techniques with physically motivated filtering. Using approximate frequency information, we identify the brightest transitions and extract only these important modes from the time propagation. By doing so, we effectively precondition the problem for super-resolution, reducing the number of required time steps for signal reconstruction to a minimum. We demonstrate our approach on systems containing several hundred heavy atoms, achieving up to 20-fold speedups while maintaining spectral accuracy even for signals dominated by large continua.

MM 37.3 Thu 16:15 SCH/A315

Electron thermalization in TDDFT and Ehrenfest molecular dynamics — •Tobias Zier, Uday Panta, and David A. Strubbe — University of California, Merced, USA

A non-equilibrium electronic state will in general thermalize toward an equilibrium state due to electron-electron interactions as well as interactions with ions. The description of such processes has remained unclear and controversial in time-dependent density functional theory (TDDFT), given that the occupation numbers remain fixed over time and that adiabatic functionals do not include explicit dissipation. Nevertheless in the literature signs of thermalization to a Fermi-Dirac distribution have been found in effective occupations constructed by projection of the time-dependent wavefunctions onto the ground state. Key issues include whether this process is physical or an artefact, connection to the Eigenstate Thermalization Hypothesis, and the dependence on the density of states, external fields, and xc functionals. To shed light on these phenomena, we study explicit time propagation of graphene after ultrafast laser pulses, with the Octopus real-space code, with and without ionic motion in Ehrenfest molecular dynamics. We study oscillations and the approach to an effective Fermi-Dirac distribution as well as decay of off-diagonal density matrix elements. This work has implications for treatment of statistical mechanics in a TDDFT framework and the nature of time-dependence in xc functionals, as well as for practical calculations of light-matter interactions especially for strong fields as in laser fusion experiments leading to warm dense matter and plasmas

MM 37.4 Thu 16:30 SCH/A315

Bulk plasmons in elemental metals — •Claudia Cardoso[1], Dario Leon[2], and Kristian Berland[2] — [1]S3 Centre, Istituto Nanoscienze, CNR, 41125 Modena, Italy — [2]Department of Mechanical Engineering and Technology Management, Norwegian University of Life Sciences, NO-1432 Ås, Norway

We have developed an effective analytical representation of the main collective excitations of the dielectric response of 26 elemental metals, starting from first principles calculations. Spectral band structures are then constructed , by extending our earlier model based on multipole-Padé approximants (MPA) [1,2] to incorporate both momentum and frequency dependence (MPA(q)). With this representation, we are able to identify plasmonic quasiparticle dispersions exhibiting complex features, including non-parabolic energy and intensity dispersions, discontinuities due to anisotropy, and overlapping effects that lead to band crossings and anti-crossings. We find good agreement with available experimental data. The results for elemental metals and their effective MPA(q) representation establish a reference point that can guide both fundamental studies and practical applications in plasmonics and spectroscopy.

[1] D. A. Leon, C. Cardoso, T. Chiarotti, D. Varsano, Phys. Rev. B 104, 115157 (2021).

[2] D. A. Leon, A. Ferretti, D. Varsano, E. Molinari, and C. Cardoso, Phys. Rev. B 107, 155130 (2023).

MM 37.5 Thu 16:45 SCH/A315

Probing the influence of core-hole and atomic multiplets in the final states on L2,3 edges for high-throughput studies — •Prathibha Chandrashekhar, Felix Sorgenfrei, Patrik Thunström, Olle Eriksson, and Heike C. Herper — Department of Physics and Astronomy, Uppsala University

Core level spectroscopy like X-ray absorption spectroscopy and the corresponding X-ray magnetic circular dichroic signals are powerful tools to study a wide variety of element specific properties in materials. In this work, we use ab initio density functional theory (as implemented in RSPt[1]) with multiplet ligand field theory to simulate the spectra by constructing and solving the single impurity Anderson model. We simulate the $L_{2,3}$ edges of transition metals in Heusler alloys, aiming to explore the suitability of the method for future high throughput studies, we look at $CoFeMnSi$ and Ni_2MnGa as our initial test cases. These alloys have been extensively studied for their fascinating tunable electronic and magnetic properties which find applications in spin resolved conductance devices, magnetocalorics and spintronics. We test the influence of Slater-Condon parameters on the spectra. We show that the final state effects are crucial in observing the fine structure and the branching ratio between the edges. This work is funded by Horizon Europe MSCA Doctoral Network grant n.101073486, EUSpecLab, funded by European Union. [1] RSPt, Relativistic Spin Polarized Toolkit (2017).