

Report on
Correlation Meeting
8-9 Dec. 2014
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This discussion meeting on correlation has confirmed the success of its format, as shown by the high number of participants, the high percentage of participants who attended already the previous meetings, and the growing enthusiasm and interest of the scientific community around these kind of meetings.

In this edition we got seven talk (see program), which took on average 1 and 1/2 hour each, thanks to plenty of time devoted to questions and discussions.

We started with two talks on the electron-nuclear coupling, how to treat it beyond the Born-Oppenheimer approximation and beyond the standard non-adiabatic approximations (Hardy Gross), and how electron correlation influences the electron-phonon coupling (Claudio Attaccalite).

We have then discussed on how electron correlation influences spin-wave excitations (Arno Schindlmayr). Various DFT-based approaches are available and one can compare them by looking at the spin-polarized homogeneous electron gas for which analytically or numerically exact results are available.

We continued with approaches beyond DFT, such as Many-Body Perturbation Theory (MBPT) and Dynamical-Mean Field Theory. Thomas Aryal showed how to introduce local vertex corrections (correlation effects beyond mean field theories) which can better capture the physics of Mott insulators (i.e. open the band gap in so-called strongly correlated systems, for which standard approximations tend to fail). In the same spirit, other two talks on how to go beyond standard approximations in time-dependent DFT and MBPT have followed. Rex Godby discussed exactly solvable models in order to understand the exact features of exchange and correlation effective potentials and Robert van Leeuwen illustrated a diagrammatic technique to get the simpler set of vertex corrections which guarantees positive photoelectron spectra.

We have finally finished with a more applied talk, about core spectroscopy and how some assumptions in commonly used methods can be lifted to improve the physical description.

In conclusion, lots of progress have been done in the comprehension of limitations of standard methods to describe electron correlation and several new ideas have been proposed to go beyond these approximations. It is clear that this step is necessary, but the way to take it is not unique. One risks to deal with very complicated equations which, if in principle or for simple model systems can be solved, are out of reach for real systems. Therefore one has to be clever and look for that idea (or those ideas) which combines accuracy and feasibility.

Confirmed Participants:

Thomas Aryal	Hardy Gross	Claudia Rödl
Ferdi Aryasetiawan	Giovanna Lani	Davide Sangalli
Claudio Attaccalite	Robert van Leeuwen	Mark van Schilfgaarde
Silke Biermann	Lucie Prussel	Arno Schindlmayr
Sophie Chauvin	Giovanni Onida	Francesco Sottile
Guido Fratesi	John Rehr	Lorenzo Sponza
Christoph Friedrich	Lucia Reining	Nicolas Tancogne-Dejean
Giorgia Fugallo	Igor Reshetnyak	Walter Tarantino
Matteo Gatti	Dario Rocca	Marilena Tzavala
Rex Godby	Pina Romaniello	Sky Zhou

MONDAY 08-12-2014

Hardy Gross: [Introduction to electron-nuclear coupling](#)

Claudio Attaccalite: [Correlation and electron-phonon coupling](#)

Arno Schindlmayr: [Magnetic spin-wave excitations](#)

Thomas Aryal: [A local, dynamical and self-consistent approximation to Hedin's three-leg vertex to unify the fluctuation-exchange and Mott pictures](#)

TUESDAY 09-12-2014

Rex Godby: [Exact correlation in small model systems from propagation of the TDSE](#)

Robert van Leeuwen: [Vertex corrections](#)

Guido Fratesi: [Core Spectroscopies](#)