Correlation Meeting

Palaiseau, Ecole Polytechnique, 5-6 December 2011

F.Sottile
LSI, Ecole Polytechnique, Palaiseau
francesco.sottile@polytechnique.fr

P.Romaniello
LPT, Universite de Toulouse
pina.romaniello@irsamc.ups-tlse.fr

1. Proposal

1.1 Introduction and motivation

The description, comprehension, and prediction of the effects of electron correlation in real materials is nowadays one of the greatest challenges for the theoreticians of condensed matter. Correlation is responsible for a great variety of effects such as the superconductivity or the adhesion of a gecko on a surface. The difficulty lies in the fact that one deals with so-called many-body phenomena, intrinsically due to the interaction among all the (10^{23}) electrons in a system. The existing approaches allowed us to advance the comprehension, and even to describe a wide range of materials in a realistic way. Nevertheless, the present level of approximations does not provide yet with a predictive theory that can design materials without relying too much on hypotheses. Discussion meetings dedicated to the first principles treatment of correlation are envisaged in order to access the true limit of the current approaches, identify common "grand challenges", stimulate further developments.

We plan to gather people from various groups working in this domain and willing to have an informal, pedagogical and fruitful discussion. The meeting is intended to be a working forum. The format will consist in a series of long detailed talks, typically 1 hour (30 mn talk + 30 mn for questions) focusing in particular on ongoing problems and open ends. Some free time will furthermore be reserved for collective discussions. We thus urge participants to prepare their talks in this spirit.

1.2 State of the art

Today state-of-the-art for electronic structure calculation is given essentially by two approaches: the Density Functional Theory (DFT) with its non-equilibrium extension Time Dependent DFT (TDDFT); and the Many Body Perturbation Theory (MBPT). Both theories, in principle exact, presents advantages and drawbacks when it comes to practical applications, for many approximations, assumptions, restrictions come to play.

Today's most successful methods rely on a smart combination of DFT and MBPT, to combine the relative numerically low-cost of DFT, with the accuracy of Many-Body Approaches, like GW approximation, Bethe-Salpeter equation, or Dynamic Mean Field Theory.

Great interest has been given in the last decade to transition metal oxides, often called strongly-correlated materials, both for their intrinsic complexity that makes their study intellectually challenging (also offering severe tests for the theory) and for the prospect of novel applications (high-Tc superconductors, colossal magneto-resistance, transparent conducting materials, etc.)

We plan, for the present Discussion Meeting, to tackle both the theoretical and numerical approaches for the description of different class of correlated materials.

1.3 Objectives

The aim is to gathered together several experts in complementary fields, all related to certain aspects of electron correlation: magnetic materials, DMFT, theory developments, GW+BSE, TDDFT are only some of the topics that could be covered by the 15-20 participants who have agreed (almost all of them already gave their OK to participate) to participate at the Meeting next December.

The topics chosen for this meeting, for which different contributions and different points of view are expected are:

- satellites in photo-emission spectroscopy and numerical techniques to describe them (DMFT, self-consistent GW, cumulant expansion)
- Band-Gap problem in strongly correlated systems. Beyond GW: starting point and vertex corrections
- Charge transfers plasmons and satellites.

We plan to start the meeting on Monday morning and end it on the following Tuesday late afternoon. The participants can then arrive on Sunday evening and leave on Wednesday morning. A tentative program is thus :
Day 1 (Mon) : 08 :30 - 13 :00 (4 × 1 hour + 1 coffee break)
Day 1 (Mon) : 14 :30 - 18 :00 (3 × 1 hour + 1 coffee break)
Day 2 (Tue) : 08 :30 - 13 :00 (4 × 1 hour + 1 coffee break)
Day 2 (Tue) : Discussion session in the afternoon.

1.4 Participant List

Angel Rubio, Universidad del País Vasco, Spain (angel.rubio@ehu.es)
Matteo Gatti, Universidad del País Vasco, Spain (matteo.gatti@ehu.es)
Patrick Rinke, Fritz-Haber Institute, Berlin, Germany (rinke@fhi-berlin.mpg.de)
Xinguo Ren, Fritz-Haber Institute, Berlin, Germany (ren@fhi-berlin.mpg.de)
Fabio Caruso, Fritz-Haber Institute, Berlin, Germany (casadei@fhi-berlin.mpg.de)
Antoine George, École Polytechnique, Palaiseau, France (antoine.georges@polytechnique.edu)
Silke Biermann, École Polytechnique, Palaiseau, France (silke.biermann@polytechnique.edu)
Lucia Reining, École Polytechnique, Palaiseau, France (lucia.reining@polytechnique.edu)
Giovanna Lani,École Polytechnique, Palaiseau, France (giovanna.lani@polytechnique.edu)
Claudia Rödl, École Polytechnique, Palaiseau, France (roedl@theory.polytechnique.fr)

Matteo Guzzo, École Polytechnique, Palaiseau, France (matteo.guzzo@polytechnique.edu)
Arjan Berger, École Polytechnique, Palaiseau, France (arjan.berger@polytechnique.edu)
Hardy Gross, Fritz-Haber Institute, Halle, Germany (hardy@mpi-halle.mpg.de)
John Rehr, University of Washington, Seattle, USA (jjr@uw.edu)
Rex Godby, Departement of Physics, University of York, UK (rwg3@york.ac.uk)
Friedhelm Bechstedt, University of Jena, Germany (bech@ifto.physik.uni-jena.de)
Andreas Schrön, University of Jena, Germany (andreas.schroen@uni-jena.de)
Ulf von Barth, University of Lund, Sweden (barth@teorfys.lu.se)

2. Financial Support

We ask CFCAM a support for this Meeting, of the order of 3000 €, to cover logistic expenses, like coffee breaks (~500€), lunches for the participants coming from abroad (~500€), and travel expenses for selected young participants.
A local support will be given by the École Polytechnique.
The European Theoretical Spectroscopy Facility fund the travel expenses of the senior researchers and professors attending the Meeting.