Correlation Meeting

Palaiseau, École Polytechnique, 8-9 December 2014

Organisers

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1. Proposal

1.1 Introduction and motivation

Following the successful discussion meetings on Correlation held at the École Polytechnique in December 2012 and 2013 and supported by CFCAM, also this meeting aims at stimulating constructive discussions, collaborations, and knowledge exchange among a selected group of theoreticians.

Electronic correlation will play again the leading role in this discussion meeting. Its theoretical description is one of the great challenges in condensed matter physics, and much effort is dedicated in understanding the limits of the currently used approximations and proposing new ones. Many progress have been made, but still advances are needed, in particular with the discovery/application of new materials which exhibit a wealth of extraordinary complex physics. In this case exchange of knowledge and combination of successful ideas may lead to real progress.

Therefore 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, present advantages and drawbacks when it comes to practical applications. In principle one would like to combine together the relative numerically low-cost of DFT, with the accuracy of Many-Body (MB) Approaches, like GW approximation, Bethe-Salpeter equation, or Dynamic Mean Field Theory. However, also MB methods show some shortcomings and more accurate approximations are then needed, in order to describe the wealth of emergent new physics.

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

One way to go beyond the standard methods is to try to correct some basic shortcomings that plague them. Tremendous progress has been made in recent years to understand why current approximations fail in certain situations. This has been done, for example, by studying models that are exactly solvable. This understanding helps greatly to make physically motivated approximations with which to calculate real systems, but also elucidates the origin of possibly unphysical results

that one can obtain in calculations.
In the present Discussion Meeting we plan to tackle some fundamental theoretical aspects as well as computational aspects 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 have already confirmed their participation) 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:

- Dynamical effects in transition metal oxides: plasmon satellites, hole-hole satellites, multiple excitations
- H_2 dissociation (DMFT, self-consistent GW, cumulant expansion, T-matrix, Density matrix)
- Multiple solutions in GW and beyond

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

1.4 Participant List

- **Arjan Berger**, École Polytechnique, Palaiseau, France (arjan.berger@polytechnique.edu)
- **John Rehr**, University of Washington, Seattle, USA (jjr@uw.edu)
- **Silke Biermann**, École Polytechnique, Palaiseau, France (silke.biermann@polytechnique.edu)
- **Fabio Caruso**, Fritz-Haber Institute, Berlin, Germany (caruso@fhi-berlin.mpg.de)
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- **Pierluigi Cudazzo**, Universidad del País Vasco, Spain (pierluigi.cudazzo@ehu.es)
- **Kay Dewhurst**, Max Planck Institute, Halle, Germany (dewhurst@mpi-halle.mpg.de)
- **Matteo Gatti**, Universidad del País Vasco, Spain (matteo.gatti@ehu.es)
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- **Hardy Gross**, Max Planck Institute, Halle, Germany (hardy@mpi-halle.mpg.de)
- **Matteo Guzzo**, École Polytechnique, Palaiseau, France (matteo.guzzo@polytechnique.edu)
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- **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.