CECAM – ESF Workshop on:
"Quantum Transport and non-adiabatic electron evolution from first principles approaches"

Organizers:

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Summary:

This joint CECAM – Psi-k workshop was devoted to the discussion of the theory of phase coherent electronic transport by means of first principles theories and computational methods. The workshop brought together many of the most important theorists in the area, from two differnet communities: the one of spin transport in layered solid state structures, and the one of nano- and molecular electronics. The workshop had a reduced format, as usual in CECAM events, with plenty of time for open discussion and exchange of ideas. The main conclusion of the workshop was that this is a mature field, where the basic methods are well established, but where new ideas based on time-dependent theories to describe transient and frequency dependent phenomena, and many-body theories to describe effects beyond independent electron approximations are still very much needed, and are a subject of intense current research.

Scientific Content and Discussion:

The experimental study of phase coherent transport in inhomogeneous, hybrid systems has in the last decade stimulated much effort to devise first-principles theories and computational methods capable of describing electronic transport in such situations where conventional approaches fail. Two distinct fields have developed in parallel, with little interaction; the first is largely concerned with the transport of spins in layered structures in which one or more of whose components is ferromagnetic (giant and tunnelling magnetoresistance, spin injection etc.); the other is the newer field of nanoelectronics and molecular electronics. The challenges in both areas are many, starting from an appropriate first-principles formulation of electrons out of equilibrium, up to the computational details of dealing with open systems. ”Straightforward” application of Density Functional Theory (DFT) -using the common XC functionals developed for the ground state- for the study of ballistic conduction in the nanoscale is now routinely done by many groups, and several codes have been developed for these calculations. However, a practical, well-founded theory of electrons out of equilibrium with the same level of rigor as Density Functional Theory for the ground state is still missing, and progress in this direction is very much needed. Time-dependent DFT methods are possible ways that some groups are exploring. Also, more subtle processes involving relativistic effects (responsible for some interesting processes in spin devices), inelastic effects (including electron-phonon and electron-electron interactions), and non-adiabatic processes are much more difficult to simulate, and methods for dealing with them are at their infancy.

The workshop aimed at identifying the most pressing current problems and determining the most interesting routes to solve them. This is a rapidly developing field in which rapid progress is being made in many directions. Just a very few years ago, the calculation of ballistic conductance was out of the reach of first principles methods, while nowadays there are several different codes (including commercial ones) that allow quite detailed calculations to be performed. As the computational methods advance quickly, so does the basic theory behind these calculations.

An important aim was to bring together the two separate transport communities: that of spin transport in solid state, layered structures, and that of nanoelectronics. These communities, though using fundamentally very similar techniques, have thus far had very little interaction. This interaction was very beneficial for the overall advance of the field of modeling of electronic transport. In particular, there was plenty of discussion to (i) determine which are the most interesting routes to solve the current problems, and (ii) open a channel of communication between the two communities, and learn mutually from the techniques and methods developed by each other.

Emphasis was given to both fundamental and computational aspects. We also focused on applications of existing methodologies to specific problems, including nanoelectronic devices, spintronics, tunneling in solid state devices, etc. The workshop covered both fundamental and computational aspects. The topics which were be covered included:

- NEGF and related approaches
- Non-adiabatic effects
- Time-dependent DFT and related approaches
- Other methods beyond DFT
- Molecular electronics
- Tunneling barriers
- Spin transport: spintronics, magnetoelectronics

Results and impact on the future direction of the field

The workshop was extremely lively and worthwhile, with much discussion and exchange of ideas. From the amount of new work presented, it was clearly timely, and the field is obviously still in a state of flux. The meeting of two communities (roughly characterized by their interest in different areas: either molecular electronics and narrow constrictions, or layered materials and spin transport) was profitable as it allowed the mixing of ideas and assumptions from each area.

One of the topics addressed was the calculation of transport from DFT in both communities (using Landauer approach and both scattering and non-equilibrium Green's function formalisms). This overall framework is becoming well-understood, but it is clear that there are still considerable efforts underway in the areas of efficiency and implementation. However, in a way, the workshop has established that, despites differences in the technical details of particular implementations, the basic formulation for transport based on DFT is well established and commonly accepted by both communities, who have arrived in parallel to essentially the same conceptual framework. In that sense, it seems that the workshop has arrived at a late moment, and that if it would have taken place some time ago, it would probably have had a larger impact in the development of both communities.
Going beyond these standard techniques was a major concern of the workshop. The two main topics were going beyond DFT (more accurate techniques such as GW, CI, and TDDFT to allow more precision in the calculation of the electronic structure), and including non-adiabatic effects (allowing the electronic subsystem to couple to the phononic subsystem to exchange energy). While there have been steps forward in both these areas, they are in their infancy, and the best ways to proceed are not clear. These are lines which will most probably develop quickly in the near future.

The fact that DFT approaches coupled to Non-Equilibrim Green's Functions techniques have become standard in dealing with transport problems, has lead to the community to a deep discussion of what are the limitations, deficiencies and basic flaws of these approaches. Hints on the inability to describe common effects such as Coulomb blockade have become apparent, and the basic reasons unraveled. Approaches to solve these deficiencies are being proposed. Ultimately, methods based on sound foundations like TDDFT appear to be promising, at least to understand the origin of the flaws of the standard approaches. Converting them into practical, accurate and predictive tools which can be applied to real problems is one of the main challenges for the future.

A main conclusion of the workshop was the need to find experimental validation for the quality of present-day calculations. While accurate and reliable experimental results in well controlled systems are widely available in the field of transport in solid state layered systems, the situation in the molecular electronics area is very different. There, the dispersion in the experimental results is very large (sometime, with orders of magnitude difference), as well as the difference between theory and

experiment (especially in the low-conductance regime). Having well controlled, reproducible experimental results would be extremely useful for the simulation community, in order to establish the validity and accuracy of the computational techniques.

Final Program of the Meeting:

Day 1: Dec. 04 2006

Session: 0 - Welcome and Foreword

08:50 to 09:00 : Welcome

Session: 1 - Transport in the Linear Response Regime (I)

09:00 to 09:45: **First-principles scattering matrices for spin-transport**
Maciej Zwierzycki
09:45 to 10:30: **Multilayer transport calculations within the CPA including vertex corrections**
Karel Carva
10:30 to 11:00: Coffee Break
11:00 to 11:45: **Finite element implementation of NEGF for nanostructures**
Martti Puska
11:45 to 12:30: E**lectronic transport through Wannier functions: from molecular to solid state systems**
Arrigo Calzolari
12:30 to 14:00: Lunch Break

Session: 2 - Transport in the Linear Response Regime (II)

14:00 to 14:45: **All-electron calculations of electronic transport: applications to magnetic tunnel junctions**
Daniel Wortmann
14:45 to 15:30: **Electronic transport through quantum wires and tunnel junctions: a real-space finitedifference approach**
Petr Khomyakov
15:30 to 16:00: Coffee Break
16:00 to 16:45: **Korringa-Kohn-Rostoker Green-function formalism for ballistic transport**
Phivos Mavropoulos
16:45 to 17:30: **Computing conductances by layer-KKR: from planar tunnel junctions to STM**
Jürgen Henk
17:30 to 18:00: Discussion
18:00 to 19:00: Poster Session

Day 2: Dec. 05 2006

Session: 1 - Non Equilibrium Green's Functions Approaches

09:00 to 09:45: **Ab-initio TB-LMTO method for nonequilibrium electron transport in nanosystems**
Sergey Faleev
09:45 to 10:30: **The TranSIESTA/ATK method**
Jeremy Taylor
10:30 to 11:00: Coffee Break
11:00 to 11:45: **Strong correlation and order-N in quantum transport: the Smeagol project**
Stefano Sanvito
11:45 to 12:30: **Nanoelectronics with ALACANT: Fundamentals and applications**
Juan José Palacios
12:30 to 14:00: Lunch Break

Session: 2 - Spin Transport (I)

14:00 to 14:45: **First-principles scattering matrices in magnetoelectronics**
Gerrit E. W. Bauer
14:45 to 15:30: **Ferroelectric and Multiferroic Tunnel Junctions**
Evgeny Tsymbal
15:30 to 16:00: Coffee Break
16:00 to 16:45: **Efficient spin injection from a ferromagent into a semicondutor**
Volodymyr Karpan
16:45 to 17:30: **First-principles calculations of spin-dependent tunneling and spin-disorder resistivity**
Kirill Belashchenko
17:30 to 18:00: Discussion
18:00 to 19:00: Poster Session

Day 3: Dec. 06 2006

Session: 1 - Non-adiabatic effects

09:00 to 09:45: **First principles description of inelastic transport in atomic and molecular wires**
Magnus Paulsson
09:45 to 10:30: **Open boundaries and the CEID formalism**
David R. Bowler
10:30 to 11:00: Coffee Break
11:00 to 11:45: **Correlated Electron-Ion Dynamics in molecular systems**
Andrew Horsfield
11:45 to 12:30: **Time-domain ab initio studies of ultrafast excitation dynamics in nanomaterials**
Oleg Prezhdo
12:30 to 14:00: Lunch Break

Session: 2 - Beyond NEGF DFT

14:00 to 14:45: **The flow of molecular orbitals driven by gate or bias voltage in transport calculations based on density functional theory**
Ferdinand Evers
14:45 to 15:30: **Avoiding self-repulsion in density functional description**
Roi Baer
15:30 to 16:15: **Sources, sinks and correlations in electron transport**
Giorgos Fagas
16:15 to 16:45: Coffee Break
16:45 to 17:30: **GW approach to quantum transport in nano-scale contacts**
Kristian Thygesen
17:30 to 18:15: **Linear response formalism for conductance of planar junctions**
Peter Bokes
18:15 to 19:00: **Hydrodynamic approach to transport in nano-systems**
Roberto D'Agosta
19:00 to 20:00: Discussion

Day 4: Dec. 07 2006

Session: 1 - Spin Transport (II)

09:00 to 09:45: **Interface resistance calculated from first principles approaches**
Ke Xia
09:45 to 10:30: **Spin-transport calculations in magnetic materials with presence of spin-orbit coupling and disorder**
Anton Starikov
10:30 to 11:00: Coffee Break
11:00 to 11:45: **High TMR ratio in Fe/MgO/Fe junctions with even one atomic Fe layer**
Peter Zahn

Session: 2 - Molecular Electronics

11:45 to 12:30: **The physics and chemistry of molecular devices for moletronics and for the post CMOS era**
Jorge Seminario
12:30 to 14:00: Lunch Break
14:00 to 14:45: **Applications of the Smeagol code to atomic and molecular junctions**
Jaime Ferrer
14:45 to 15:30: **First-principles calculation for electron conduction properties using real-space finite-different method**
Tomoya Ono
15:30 to 16:15: **Conductance, surface traps and passivation in doped silicon nanowires**
Marivi Fernandez-Serra
16:15 to 16:45: Coffee Break
16:45 to 17:30: **Impurities in atomically-thin metallic nanowires**
Frederico Novaes
17:30 to 18:15: **Quantum Transport in Post-CMOS Molecular Materials & Devices:**
Stefan Roche
18:15 to 19:15: Discussion

Day 5: Dec. 08 2006

Session: 1 - Time Dependent DFT Approaches

08:30 to 09:15: **Long-time dynamics of the Kohn-Sham system for open molecular junctions**
Gianluca Stefanucci
09:15 to 10:00: **Time-Dependent Transport Phenomena: Transients, Pumping and the Role of Bound States**
Stefan Kurth
10:00 to 10:45: **Classical Nuclear Motion in Quantum Transport**
Claudio Verdozzi
10:45 to 11:15: Coffee Break
11:15 to 12:15: Discussion

12:15 to 12:20: Closing word