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# SEMINAIRE

## Lundi 13 Novembre 2006 à 11h00

## Bâtiment 466, salle 111 - CEA Saclay, 91191, Gif sur Yvette

# New approach to first-principles calculations on non-equilibrium electronic systems


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Invité par M.C. Desjonquères


**Abstract:**

Electron correlation plays an important role in the dynamics of systems both in and out of equilibrium. In this talk, I will discuss how to include these effects in first-principles calculations. For calculations on steady-state systems, such as, e.g., conduction through a single-molecule device, approaches based on density functional theory are commonly used, but it is very difficult to improve the description of electron correlation effects in non-equilibrium systems beyond the very crudest approximations. Non-equilibrium Green function techniques are in this respect useful, both for constructing improved density functionals, and for providing benchmark results for testing new functionals. These methods have the advantage that the approximations can be improved systematically by diagrammatic techniques. Long thought to be merely a formal device, it is indeed possible to propagate the Green function in time also for inhomogenous systems, and in the presence of an arbitrarily strong applied time-dependent potential. I will demonstrate this by some examples for atoms and molecules. Not only is a large number of observables directly given by the Green function, but the results have the advantage of being unambiguous, internally consistent, and in agreement with macroscopic conservation laws. A property of particular interest is excitation energies, for which time-propagation is equivalently to solving the Bethe-Salpeter equation with a highly sophisticated kernel. The method is very general, and is applicable for larger system within the framework of model Hamiltonians. I will further discuss potential applications of the propagation techniques, which are well suited for systems such as quantum dots and polymers. I will indicate how non-equilibrium Green function techniques serve as a complement to time-dependent density functional theory, and for this reason will be highly useful for developing improved methods for realistic calculations on larger systems.


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