Dottorato di Ricerca in Fisica dell'Università degli Studi di Messina

11 Giugno 2012, ore 15.00, Aula E. Majorana, Dip.to di Fisica,
V.le F. Stagno d'Alcontres 31, S. Agata, Messina

Seminar title:

Nonadiabatic dynamics of quantum-classical systems

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Abstract

Nonadiabatic quantum dynamics takes place when coupled physical systems are free to exchange energy during their time evolution.
This happens almost ubiquitously in condensed matter physics.
In this talk, various examples of nonadiabatic dynamics will be presented and the issues faced by its numerical simulation will be discussed.
Typically, unavoidable limitations of the computational power make it impossible to perform a full quantum simulation of the dynamics of general interacting manybody systems.
However, when one is only interested in quantum effects on a small part of the total system, a hybrid quantum-classical approach can be used.
Even in this case, both the formulation and the implementation of nonadiabatic dynamics are very difficult.
Starting from quantum mechanics, It will be shown how quantum-classical nonadiabatic dynamics can be formulated by means of a number of controlled approximation in a partial Wigner representation.
As for the implementation of nonadiabatic dynamics,it will be illustrated how the growth of the statistical error at long times can be tamed by a generalized sampling scheme.