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It may be said that in every attentive look on nature we already theorize. But in order to guard against the possible abuse of this abstract view, in order that the practical deductions we look to should be really useful, we should theorize without forgetting that we are so doing, we should theorize with mental self-possession, and, to use a bold word, with irony.

W.G.

Publications and Reprints

Research Interests

My work has focused mainly on developing simulation methods for studying condensed phase systems that exhibit quantum characteristics, with particular reference to non-adiabatic effects in the dynamics. In that connection, during my Ph. D., I have improved the numerical efficiency of existing semiclassical non-adiabatic methods by taking advantage of some formal properties of the mapping hamiltonian formalism for describing electronic transitions. Combining the mapping formalism with a well defined approximation of the path integral expression for quantum time correlation functions, I have also developed a novel mixed quantum-classical approach, called LAND-Map, for calculating such quantities. When applied to realistic models of condensed phase systems, and in particular to the diffusion properties of an excess electron in a metal-molten salt solution, this approach has proved considerably more efficient than other existing methods and very accurate. Recently, I have started studying systems of biological interest with the intent to combine coarse grained methods with non-adiabatic approaches of the kind described above. This would allow one to address, for example, the photophysical properties of a small quantum subsystem, such as a chromophore, embedded in a protein represented in a coarse grained scheme. In collaboration with my colleagues at the Scuola Normale Superiore, I have also developed a new method for the statistical analysis of protein alignments that helps to identify specificity determining residues in families of homologous proteins. The method has been successfully applied to recognize amino acids relevant in achieving a functional monomerization of the DsRed tetrameric protein.

Current Research Projects

- **Hydrogen storage in solid state materials**

Finding a safe, convenient, and efficient way to store hydrogen is one of the major problems in current attempts to substitute fossil fuels with sustainable energy sources. Solid state storage materials have emerged as interesting candidates in this field, but a better understanding of their structural and thermodynamic properties is necessary before they can be used in technological applications. Several experiments indicate that alanates, a class of aluminum and light-metals hydrides show particular promise. The existing studies, however, are unable to resolve a number of ambiguities in the hydrogen capture and release mechanisms in alanates

whose clarifications is key for improving their storage efficiency to satisfactory levels. The goal of this research project is to develop and apply simulation methods capable of supplementing the experiments in the study of the hydrogen storage properties of sodium alanate.

- **Mixed quantum-classical dynamics**

The numerical cost of exact methods for studying the dynamical properties of quantum systems scales exponentially with the number of degrees of freedom. Consequently, considerable effort is currently devoted to developing simulation methods that approximate the quantum evolution of the system with the necessary accuracy while reducing as much as possible the computer resources needed. A fruitful strategy developed since the 1970s to address the quantum problem via computer simulation is to partition the different degrees of freedom in two sets, usually on the basis of mass or energy ratio considerations. One of the sets, which can be quite large, is treated classically, the other, typically consisting of a small number of degrees of freedom, is described quantum mechanically. In collaboration with David Coker at Boston University, we have recently developed a new mixed quantum-classical method that is particularly well suited to compute time correlation functions. The method is called LAND-Map (Linearized Nonadiabatic Dynamics using the Mapping formalism) and it can be applied both to systems that evolve according to the adiabatic, or Born-Oppenheimer, approximation or to so called non-adiabatic problems.

Related Links

CECAM Workshop May 2007

Les Diablerets Talk

Teaching activity

Laboratorio di Calcolo 1

Meccanica Quantistica