Position: Postodoctoral fellow

Affiliation: Physics Dept. University of Rome "La Sapienza", P.le A. Moro 2, I-00185 Rome, Italy
Office: Ed. Marconi, Room 339 C
Telephone: +39 06 4969 4281
Fax: ----
Email: *federicaDOTagostiniATroma1DOTinfnDOTit This e-mail address is being protected from spambots. You need JavaScript enabled to view it*

Curriculum Vitae

Publications and Reprints

Research Interests

My work concerns with a quantum-classical approach to molecular dynamics. The development of a fully quantum molecular dynamics in condensed phases of matter is conditioned by severe computational limitations. The solution of the Schroedinger equation for a macroscopically significant number of degrees of freedom is presently out of reach. However, in many relevant problems, a full quantum description is unnecessary: there are cases in which the majority of the degrees of freedom of the system (atoms, ions, molecules) can be reasonably treated as classical, and the need for a full quantum description is limited to a small number of degrees of freedom. These are, e.g., electrons or protons whose dynamics is non adiabatically coupled to the classical molecular dynamics. In this context, the derivation of quantum-classical equations of motion, which couple many classical degrees of freedom to a small number of quantum degrees of freedom is a very relevant goal. Attempts in this direction have not produced, so far, conclusive results. Recently, a formal derivation of quantum-classical brackets has been claimed by Vladimir V. Kisil. Such a derivation is based on an alternative formulation of quantum and classical mechanics using the Heisenberg group representation theory, taht can be used to describe the evolution of two coupled systems, characterised by two different values of the Planck constant. Kisil proposed an anstatz on the equation of motion to describe the evolution of such a system, but it brings to a trivial result in the quantum-classical limit. I am actually studying a different way to formally derive quantum-classical equation of motion.

Current Research Projects

- **Quantum-classical equation of motion**

I am investigating a procedure to solve mathemathical and physical inconsistencies of Kisil's theory on quantum-classical dynamics. The starting point is once again the Heisenberg group representation theory but I would like to introduce some suitable reduced units of lenght and momentum, connecting this formulation to the quantum-classical Liouville equation proposed by G. Ciccotti, R. Kapral a D. Mac Kernan.