Research activity

My research activity started with a Non-Equilibrium Molecular Dynamics (NEMD) investigation of thermal transport coefficients for Coulomb systems. Later, during my PhD training, I studied polymer solutions always using Molecular Dynamics. After these experiences with classical fluids I addressed my research towards quantum fluids and in particular electron fluids, by employing and developing Quantum Monte Carlo (QMC) methods. However I have always followed the development in the field of classical fluids and soft matter where recently I have given interesting contributions.
I have authored 100 publications on international journals, some rather prestigious.

My research activity can be presented along two distinct lines: i) classical systems (simple and complex fluids, equilibrium and out of equilibrium properties); ii) quantum many-body systems.

1. Classical fluids and polymers

I have studied Coulomb fluids and polymer solutions at equilibrium and out-of-equilibrium, using standard Molecular Dynamics (MD) and NEMD, and Monte Carlo (MC) methods to sample the configuration space of long linear chains and to compute free energies [97, 96, 95, 94, 93, 92, 91, 90, 89, 86, 83, 82, 80, 79, 65, 62, 60, 56, 54, 53, 52, 50, 41, 40, 39, 37, 36, 35, 34, 30, 29, 27, 24, 21, 19] (the numbers refer to the list of publications enclosed below). Relevant results in chronological order are:

1. MD validation of the Zimm scaling for the dynamical relaxation of a single chain in explicit solvent (with J.P. Ryckaert) [94, 91].

2. non-linear response of dilute polymer solutions under flow of various geometries with NEMD (with J.P. Ryckaert)[89, 86, 82, 79, 95].

3. investigation of the appearance of Pincus blobs in a stretched linear chain with Configurational Biased MC (with J.P. Ryckaert et al.) [83, 80, 74].

4. development of a thermodynamically consistent, multi-scale coarse-graining strategy for solution of homopolymers and copolymers (with J.P. Hansen, A. Pelissetto et al.) [65, 62, 53, 52, 50, 41, 40, 39, 36, 35, 34, 30, 29, 27, 24, 21]

Moreover, in collaboration with an experimental group in Rome and a groups in CEA Saclay, I studied the self-assembling of nonionic surfactants in aqueous solutions by "all-atom" MD simulation [76, 71, 68, 64, 63, 59, 55]. Our specific interest was in studying the microscopic structure of the extended interface in those systems and the confining effects on the structure and dynamics of water molecules, as support to interpret experiments. The most relevant result was a study of the temperature dehydration of the interface of a spherical micelle of $C_{12}E_6$ which helped in interpreting in a coherent manner experimental results from different methods in apparent disagreement [71].

In the last three years I started investigating statistical mechanical models for actin filaments and bundles of filaments at various level of coarse-graining. The aim of this investigation is to enter in this new (to me) field with a clear theoretical framework of the biomechanics of filopodia and actin molecular motors and to try to interpret debated experiments. We have set up a clear statistical mechanical framework for a single growing filament [26], and for a bundle of filaments including the non-equilibrium properties [22, 18, 16, 11]. This work is in collaboration with J.P. Ryckaert (ULB, Belgium) and G. Ciccotti (Sapienza, Rome).

2. Many-body quantum systems

I have developed the Path Integral Monte Carlo method (PIMC) for the simulation of many-body quantum systems at finite temperature, including fermions, and I have introduced and developed a QMC-based "ab-initio" method for nuclei and electrons [88, 87, 85, 84, 78, 77, 75, 73, 72, 70, 69, 67, 66, 61, 58, 57, 51, 47, 46, 45, 44, 42, 38, 33, 32, 31, 28, 25, 23, 20, 17, 10, 15, 14, 13, 12]. This latter method, known as "Coupled Electron-Ion Monte Carlo" method (CEIMC) is the first "ab-initio" method based on correlated electron techniques which allows to study the thermodynamic behavior of systems of many electrons and ions in the Born-Oppenheimer approximation. The accuracy of CEIMC is superior to that of the standard "ab-initio" methods based on Density Functional Theory (DFT) and can be used to study physical phenomena out of reach of DFT. An example is the metallization in fluid phase. The system to which I have devoted most of my effort is the hydrogen at high pressure which has a reach physics still largely unknown.
The most relevant results obtained in this field, in chronological order, are:

1. the development of PIMC for a mixture of protons and electrons and the first PIMC study of hydrogen phase diagram at high pressure and temperature (with D.M. Ceperley et al.) [88, 87, 85, 84] .

2. the development of PIMC for Fröhlich polarons and the study of the single polaron free energy (with S. Ciuchi et al.) [78, 77].

3. the development of a systematic method to improve trial wave functions in the ground state QMC (with D.M.

Ceperley et al) [73, 58].

4. the introduction of an efficient sampling algorithm for Reptation MC, known as "the bounce algorithm" (with D.M. Ceperley) [70].

5. the introduction and development of the CEIMC (with D.M. Ceperley) [75, 72, 69, 67, 66, 61, 58, 47, 45, 44, 42, 38, 32, 31, 28, 25, 23, 20, 17, 10, 12].

6. the first "ab-initio" quantitative study, by free energy methods, of the demixing phenomenon in hydrogen-helium mixtures in thermodynamic conditions interesting to planetary physics [51].

7. the "ab-initio" study (both BOMD and CEIMC) of the metallization and molecular dissociation in liquid hydrogen under pressure [66, 46, 32, 23, 17, 10, 15, 14, 12].

Computing dynamical properties of quantum many body systems is still an open problem with modern computational methods, even for systems of few degrees of freedom. In general computing real time correlation functions requires an amount of computer time which scales exponentially with the number of degrees of freedom. The problem is very different if the system is in the semiclassical regime or near its ground state. In the former case the starting point is a Path Integral formulation and one introduces stationary phase or a linearization approximation in the real time dynamics, in the latter case one needs a methods to compute the first low-lying excited states participating into the dynamics.
My contributions in this area are:

1. the introduction of a Wigner-Liouville formalism in the semiclassical approximation (with G. Ciccotti et al.) [81].

2. the development of a mixed imaginary time Path Integral-linearized real time dynamics method for time correlation functions (with S. Bonella and G. Ciccotti) [48, 49].

3. the application of a Projection QMC method for low energy excited states (many-body) to compute the electrical conductivity of high pressure hydrogen (with D.M. Ceperley et al.) [57].

In the last years I have developed a method to compute electronic band gaps by Grand-Canonical Quantum Monte Carlo. This method solves the infamous gap problem present in the DFT formulation and provide benchmark gap values for less fundamental theories[9]. Moreover it can be easily applied to disordered systems, like quantum crystals and liquid [8]. We are presently extending the approach to compute optical properties with QMC accuracy [10, 57]