Single-particle dynamics in classical and semi-classical fluids

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An important branch of liquid state physics aims at the characterization of the microscopic dynamics of Boltzmann liquids, both classical and semi-classical, over different length (l=2π/Q) and time (t=2π/ω) scales, focusing on either collective or single-particle (*self*) properties [1, 2]. The use of different investigation techniques, like thermal neutron scattering and classical and quantum molecular dynamics simulations, has led to significant progresses over the last decades, but yet some fundamental aspects of the dynamical behavior of these liquids are still not well established.

The objects of the analysis are time correlation functions of microscopic variables and their frequency spectra. In particular: the spectrum $S(Q, \omega)$ of the autocorrelation function of density fluctuations with wave vector Q, i.e. the dynamic structure factor, and the spectrum of the autocorrelation function of the single-particle velocity, i.e. the vibrational density of states. To perform our analysis we took advantage of present simulations techniques for the calculation of quantities of difficult experimental determination.

The aim of the project is to carry out a deep study of the *self* dynamics of different fluids. In particular, we considered a model fluid, like the Lennard-Jonesium [3], liquid metals, simple molecular liquids, and quantum liquids [4], like hydrogen. The analysis has been enriched by a recent theoretical result, which states that the spectra of correlation functions in liquids are correctly interpreted in terms of series of generalized Lorentzian modes [5, 6]. This new approach has revealed not only strong similarities among all the afore-mentioned liquids, as regards the basic diffusive and vibrational processes, but also interesting connections between different dynamical spectra.

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