Quantum Hydrodynamics for Plasmonics and Nanophysics

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Recent years have witnessed a remarkable surge of interest for the electronic properties of new materials, particularly when excited by electromagnetic radiation. This is a very vast domain of research that encompasses all sorts of nano-objects (metallic films and nanoparticles, carbon nanotubes, semiconductor quantum dots …), as well as meta-materials whose structure can be engineered to display some particular electromagnetic properties. Potential applications range from high-performance computing (efficient storage and transfer of information), to **nanoplasmonics**[1] (optical filters, waveguides) and even to the medical sciences[2] (biomedical tests and sensors).

The present project focusses on **metallic nano-objects**[3] and the composite metamaterials that can be constructed out of them, such as networks of interacting nanoparticles. The main goal is to study the out-of-equilibrium electron response to electromagnetic radiation. For systems containing many electrons, ab-initio methods such as the time-dependent density functional theory (TDDFT) or the Hartree-Fock equations are very costly in terms of run time and memory storage. On the other hand, many recent investigations rely on simple approaches based on improvements of the classical Mie theory.

Here, we propose to develop and implement an intermediate approach based on a set of **quantum hydrodynamic (QHD)**[4] equations, which are sufficiently simple to be run on standard computers (desktop PC, medium-sized university cluster), but contain enough physics to study the full electron response beyond the Mie model – in particular nonlinear, nonlocal, and quantum effects. The combination of flexibility and accuracy of QHD models makes them an ideal tool to investigate many open problems in the emerging field of nanoplasmonics. Using this approach, several configurations of nano-objects will be studied: dimers and trimers of metallic nanoparticles and nanorods, metal-dielectric multilayers, nanoparticles in the vicinity of a thin metal film, and arrays of nanoparticles interacting via the electric dipole force.

The candidate will develop and analyse the QHD model and adapt it to the various configurations of nano-objects to be studied. Subsequently he/she will develop the necessary computational tools to solve the QHD equations numerically, starting from the simplest geometries (e.g., spherical symmetry) and proceeding to more complex and realistic cases (e.g., networks of nanoparticles). A longer-term objective, to be at least partially realized during the PhD program, will be the implementation of an open-source standardized QHD solver for 3D nanoplasmonics.

The prospective candidate should possess good **computational skills** applied to physics problems (numerical solution of PDEs, visualization of the results, parallelization of the codes). Some **background in condensed-matter physics and/or fluid dynamics** would also be desirable.

[1] M. I. Stockman, Opt. Express **19**, 22029 (2011).

[2] X. Huang, S. Neretina, M. A. El-Sayed, Adv. Mater **21**, 4880 (2009).

[3] Yu Luo, A. I. Fernandez, A. Wiener, S. A. Maier, J. B. Pendry, PRL **111**, 093901 (2013).

[4] N. Crouseilles, P.-A. Hervieux, G. Manfredi, Phys. Rev. B **78**, 155412 (2008).