Finite temperature orbital-free calculations for hot dense matter

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Organisers

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Introduction and motivation

We propose to organize a discussion meeting in June 2011 on finite temperature orbital free methods (FTOF) for dense plasmas simulations. These techniques are based on a direct approximation of the free-energy of an electronic system in terms of the local electronic density, i.e. being a direct application of Density Functional Theory. They constitute an alternative to the widely used orbital-based Kohn-Sham formulation of DFT and are particularly well-suited for dense plasmas. These methods are now used by several groups to compute static and transport properties of hot dense matter and mixtures with codes simulating up to 10000 particles. We think that time has arrived to compare performances of different implementations and to seek for possible routes to improve both performances and relevancy. Exchanges with people dealing with OF methods in the condensed matter field would be also very profitable, particularly from the algorithmic point of view.

State-of-the-art

20 years ago a series of Cecam meetings (1988-89-90) was organized with the goal of discussing new techniques of simulation. Among the participants were P. Madden, B. J. Alder, J.-P. Hansen, E. Smargiassi, I. Stich, G. Zérah and J. Clérouin. The output was the idea of coupling a Thomas-Fermi description for electrons with a classical molecular dynamics for the ions. This coupling was done through a Car-Parrinello scheme using the density as a degree of freedom in a fictitious Lagrangian formulation [1].
Since then, *ab initio* techniques, based on the Kohn-Sham formulation of DFT, have become the tool of choice for studying material properties, from chemistry, condensed matter to dense plasmas properties. But despite the increase of computational resources, the numerical cost of this approach prevents its use in several applications, which require large numbers of particles or basis sets, such as asymmetric mixtures or hot dense matter. The orbital-free scheme of DFT offers a powerful alternative for treating such systems but suffers from some drawbacks originating principally from the kinetic energy functional. However, serious efforts to adjust these shortcomings have received renewed attention. Since the seminal work of Chacon [2], Wang and Teter [3] and Perrot [4], several attempts have been made to improve such functionals [5-7], mainly by incorporating sophisticated non-local kernels in order to reproduce the linear response regime from the free fermion gas. It is interesting to note that, despite the interest of the community in developing accurate kinetic energy functionals, much less attention has been oriented towards the inclusion of thermal

effects [8], for example by improving free energy functionals beyond the well-known finite temperature Thomas-Fermi-von Weiszäcker functional. On the numerical side, OF-DFT has been the subject of several fields of investigation. Since the OF description can be expressed in terms of a fake orbital, the square root of the electronic density, the different algorithms – developed for the orbital based picture – can be straightforwardly used to minimize the electronic energy. Nevertheless, new schemes have been proposed to exploit the intrinsic features of the OF description to obtain linear scaling like expressing all the energy terms in real space instead of going back-and-forth between real and reciprocal spaces. This scheme, coupled with non periodic boundary conditions and adaptative mesh refinement, allows for studying systems with particularly low symmetries and large number of particles [9], with million particles capabilities such as in PROFESS code [10]. Very recently, DFT calculations involving the use of an orbital free description have been also employed in a new scheme for getting physically-meaning parameters for classical force fields [11].
Let us recall that in 2002, a CECAM workshop has been organized on approximations and applications of kinetic energy functionals by T. A. Wesolowski and several international conferences were held in this domain (OF DFT symposium : OF-DFT2 2005, OF-DFT3 2008 and OF-DFT4 2010).

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Objectives

The goals of this meeting are the following:

1. To bring together researchers working on different fields of applications of FTOF DFT, to present the specific requirements of each domain and the possible crossimprovement between them;
2. To seek for the possibility of coupling FTOF methods with standard Kohn-Sham DFT codes in order to preserve the advantages of both methods depending on the physical properties involved;
3. To discuss the further developments of functionals, stressing particularly on nonzero temperature effects;
4. To expose the implementation of efficient highly parallelizable algorithms and their specificities depending on the domain of applications. The advantage of real space implementation – in comparison with reciprocal one – for orbital free representation would be pointed out;
5. To start a reflection on time-dependent electronic properties with an orbital free description;
6. To prepare a proposal for a 2012 meeting on finite temperature orbital free methods.

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