PEOPLE

MARIE CURIE ACTIONS

Intra-European Fellowships (IEF)

Call: FP7-PEOPLE-2012-IEF

FINAL REPORT

"SCDFT"

Summary report

The main objective of the “SCDFT” IEF project was to further develop and apply a novel method for the study of strongly-correlated systems in Physics and Chemistry.

In molecules, semiconductor nanostructures, or ultracold atomic gases, the interactions between the constituent particles play a very important role and they determine many of the properties of these systems. A correct treatment of the interactions is thus fundamental. Unfortunately, an accurate treatment of the interactions poses very serious challenges to all the existing approaches, which suffer different types of limitations. In some methods, the interactions are only partially incorporated, which causes these approaches to work only in some special situations. In the case of other more accurate methods, where the full interaction is considered, the numerical resolution of the involved equations becomes unaffordable when the system contains many particles, even for the most powerful available computers.

The SCDFT project is based on a formalism called Kohn-Sham Density Functional Theory (KS DFT). In principle, this popular method combines the advantages of the two types of methods mentioned above: relatively cheap numerical implementation and exactness. This is possible because the approach treats the particles as if they were non-interacting and incorporates the effects of the interactions via an effective confining-potential term that does not cause an increased numerical cost. The method is widely used in chemistry and in many areas of physics, and it has been very successfully applied to the study of many systems. Yet, there exist some interesting situations where the approach does not work properly. One of such scenarios is the case of very strong interactions (strong correlation), and this has been the object of study within the SCDFT project.

The key ingredient in KS DFT is the so-called exchange-correlation functional, for which approximations need to be made. It is well known that all the commonly-employed ones fail when applied to strongly-correlated systems: the most famous and simple example is the dissociation process of the H2 molecule. Even though hundreds of functionals exist, none is able to describe this process entirely correctly. Most of the standard methods describe properly the molecule when the two atoms are close to each other, but not in the limit of dissociation, where the strong-correlation effects become dominant. Other methods exist that describe this phenomenon correctly, but they can do this by introducing artificial physical effects that do not correspond to the real system.

In the SCDFT project, we have further developed a very promising method. It is based on the KS DFT approach, exploiting the cheap numerical cost of this approach, but for first time it is also capable of describing very accurately strong-correlation effects. The essential idea is based on the so-called "strictly-correlated-electrons" (SCE) reference system, which was originally introduced and developed by M. Seidl and co-workers. This system is the opposite counterpart of the non-interacting one of the Kohn-Sham approach: instead of having no interaction, it contains particles with maximum possible interaction under certain constraints. A consequence of this is that the effects of strong correlation, absent in all the methods based on the Kohn-Sham system, are well captured.

The most important contribution of the SCDFT project has been to develop a method where the advantages of the two reference systems are combined. In the "KS-SCE" DFT approach the exchange-correlation functional is constructed on the basis of the SCE system, this including the strong-interaction effects, but then the standard and numerically cheap equations of KS DFT are solved.

In the SCDFT project we have further developed the KS-SCE method and applied it to a collection of model systems, including semiconductor quantum wires and quantum dots, ultracold gases with dipolar interactions, and one-dimensional chemical systems consisting of ions and molecules. Our results have shown the power of the KS-SCE approach to describe strong correlation. In the particular case of the H2 molecule, the limit of dissociation is described with extremely high precision. Also, for the semiconductor-nanostructured and ultracold gases, the characteristic phenomena of wigner localization has been observed for particle numbers much larger than those affordable with other methods.

All these studies have resulted in a four papers in high-impact journals, including two "Editor's suggestion" in Physical Review Letters and Physical Review B, a regular Physical Review B article and a paper in a special issue of Physical Chemistry Chemical Physics (see the list of publications on the corresponding section).

In addition, the KS-SCE results have been presented in several international conferences in the US, France, Italy, Germany and Czech Republic, through both invited and contributed talks. In addition, the SCDFT project has contributed to increase the interest on our approach from other international groups (see, for example, C. B. Mendl and L. Lin, Phys. Rev. B **87**, 125106 (2013); H. Chen, G. Friesecke, and C. B. Mendl, J. Chem. Theory Comput. **10**, 4360 (2014); J.-D. Benamou, G. Carlier, and L. Nenna, arXiv:1505.01136v2 (2015)). At the same time, the project has initiated collaboration with the groups of Prof. S. M. Reimann (Lund University, Sweden) and C. Mendl (Standford University, US).

Finally, the project has also included two different outreach activities. The first one has been the writing of an article on the SCE formalism on Wikipedia (https://en.wikipedia.org/wiki/Strictly-Correlated-Electrons_density_functional_theory), and the second one a popular-science presentation entitled “Science in arts and arts in science” for high-school students at the Murmellius Gymnasium in Alkmaar (The Netherlands), given together with another IEF fellow from the Theoretical Chemistry department of the VU University Amsterdam.