Dixièmes Journées Franco-Chiliennes d'Optimisation
INSA Rouen Normandie, Rouen, France
8-11 July 2025

DISSOCIATION LIMITS IN DENSITY FUNCTIONAL THEORY

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In this talk we consider the Density Functional Theory (DFT) framework, where a functional of the form $F_\varepsilon(\rho) = \varepsilon T(\rho) + bC(\rho) - U(\rho)$ has to be minimized in the class of non-negative measures ρ which have a prescribed total mass m (the total electronic charge). The parameter ε is small and the terms T, C, U respectively represent the kinetic energy, the electronic repulsive correlation, the potential interaction term between electrons and nuclei. Several expressions for the above terms have been considered in the literature and our framework is general enough to include most of them. It is known that in general, when the positive charge of the nuclei is small, the so-called *ionization phenomenon* may occur, consisting in the fact that the minimizers of F_ε can have a total mass lower than m; this physically means that some of the electrons may escape to infinity when the attraction of the nuclei is not strong enough. Our main goal in this talk is to illustrate the asymptotic behavior of the minimizers of F_ε as $\varepsilon \to 0$, , continuing the research we started in [1]. In particular we obtain that the Γ-limit functional is defined on sums of Dirac masses and has an explicit expression that depends on the terms T, C, U that the model takes into account. We shall illustrate this on some explicite examples.

References

[1] G. Bouchitté, G. Buttazzo, T. Champion, L. De Pascale: *Dissociating limit in Density Functional Theory with Coulomb optimal transport cost*, Ann. Scuola Norm. Sup. Pisa Cl. Sci., 22, 1429–1471, 2021

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