

Sparse approximation of the Lieb functional in DFT with moment constraints

jeudi 7 septembre 2023 14:00 (1 heure)

(joint work with Luca Nenna)

In this talk, we will present recent mathematical results about the Lieb functional in Density Functional Theory. More precisely, the Lieb functional, for a given electronic density, can be viewed as a generalized form of optimal transport problem for which the electronic density plays the role of a marginal. A numerical discretization of this problem can be obtained by imposing a finite number of moment constraints instead of this full marginal constraints. Using the so-called Tchakhaloff's theorem, it can be shown that a minimizer of the approximate Lieb problem can be obtained as a finite-rank projector, the rank of which is at most equal to the number of moment constraints of the problem. In other words, such minimizer has a very sparse structure which can be exploited for numerics. We will highlight some open questions related to the practical resolution of such problems, which require the use of advanced methods for manifold-constrained Monte-Carlo sampling.

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Classification de Session: Challenge and Perspective