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Moment-Constrained Approximation of the Lieb functional

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The aim of this talk is to present new sparsity results about the so-called Lieb functional, which is a key quantity in Density Functional Theory for electronic structure calculations for molecules. The Lieb functional was actually shown by Lieb to be a convexification of the so-called Lévy-Lieb functional. Given an electronic density for a system of N electrons, which may be seen as a probability density on R^3, the value of the Lieb functional for this density is defined as the solution of a quantum multi-marginal optimal transport problem, which reads as a minimization problem defined on the set of trace-class operators acting on the space of electronic wavefunctions that are antisymmetric L^2 functions of R^{3N}, with partial trace equal to the prescribed electronic density. We introduce a relaxation of this quantum optimal transport where the full partial trace constraint is replaced by a finite number of moment constraints on the partial trace of the set of operators. We show that, under mild assumptions on the electronic density, there exist sparse minimizers to the moment-constrained approximation of the Lieb (MCAL) functional that read as operators with rank at most equal to the number of moment constraints. We also prove under appropriate assumptions on the set of moment functions that the value of the MCAL functional converges to the value of the exact Lieb functional as the number of moments go to infinity. Finally, we show that a semi-classical limit holds, namely MCAL \Gamma-converges to the moment constraints multi-marginal optimal transport.This is a joint work with Virginie Ehrlacher.

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