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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 defined on the set \mathbb{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 constrained approximation of the Lieb (MCAL) functional that reads as operators with rank at most equal to the number of

Joint work with Luca Nenna (Laboratoire de Mathématiques d'Orsay, France).