

# The ground state of the Dirac-Fock model: a new approach

*Wednesday, January 31, 2024 5:00 PM (50 minutes)*

I will present a new approach to the ground state of the relativistic Dirac-Fock energy inspired of Lieb's relaxed variational principle for Hartree-Fock. This approach seems simpler and more suitable for theoretical and numerical investigations than previous ones. Based on this approach, I will present existence results for the ground state of molecules and crystals. The existence proof for this ground state suggests an algorithm for its computation, that generalizes the ODA algorithm of Cancès-Lebris. The existence result for crystals is joint work with Isabelle Catto, Long Meng and Eric Paturel. The theoretical study and implementation of the algorithm is work in progress with Maxime Chupin, Guillaume Legendre and Long Meng.

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