Seminario de análisis matemático y aplicaciones
Analisi matematikoa eta aplikazioak mintegia

Accuracy of the Time-Dependet Hartree-Fock Approximation

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ABSTRACT: One of the fundamentals problems of quantum chemistry is the description of the dynamics of the electrons in a molecule. Unfortunately this problem is extremely complicated, both theoretically and from a numerical viewpoint. Approximations are thus used, one of the most fundamental being the Hartree-Fock approximation. Although it is commonly used by chemists, only few mathematically rigorous results allow to justify this approximation. I present the results of a collaboration with V. Bach and T. Tzaneteas. I introduce the mathematical model for a molecule and the approximation of its dynamics by the time-dependent Hartree-Fock equation. I state our result which gives an estimate of the quality of the approximation, along with some applications.

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