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Variational problems in Relativistic Quantum Chemistry

This talk is based on a series of joint works with J. Dolbeault, M. J. Esteban, C. Hainzl and M. Lewin, on stationary solutions of linear and nonlinear equations from Relativistic Quantum Chemistry, involving the Dirac operator. The solutions are found as critical points of an energy functional under normalization constraints. Contrary to the Laplacian appearing in the equations of nonrelativistic Quantum Mechanics, the Dirac operator has a negative continuous spectrum which is not bounded from below. As a consequence, the energy functional is strongly indefinite, i.e., all its critical points have an infinite Morse index. The associated Euler–Lagrange equations are linear or nonlinear eigenvalue problems with eigenvalues lying in a spectral gap. Moreover, since we work in the space domain $\mathbf{R}^3$, the Palais–Smale condition is not satisfied. For these reasons, the problems discussed here pose a challenge in the Calculus of Variations. The existence proofs involve sophisticated tools from nonlinear analysis and have required new variational methods which are now applied to other problems.

I will focus on the problematic definition of the "ground state" of atoms and molecules in Relativistic Quantum Chemistry, keeping in mind computational issues which are essential in this field. In nonrelativistic Quantum Mechanics, the "ground state" is simply a minimizer of the energy under normalization constraints. But in the Dirac–Fock model, which is commonly used in numerical relativistic calculations, the energy is not bounded below. Therefore the definition, existence proof and numerical computation of the "ground state" require much more care.