Title: A numerical analysis for the Coupled Cluster method used in electronic structure calculation

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Abstract:

Many properties of atoms, molecules and solid states are described quite accurately by solutions Ψ of the electronic Schrödinger equation $H \Psi = E \Psi$, an extremely high-dimensional operator eigenvalue equation for the Hamiltonian H of the system under consideration. Of utmost interest is the smallest eigenvalue of H and the corresponding eigenfunction, giving the ground state energy and the electronic wave function describing the ground state, respectively.

In the first part of this talk, the audience is introduced to the electronic Schrödinger equation and the typical problems that arise when dealing with this equation. We will then introduce the Coupled Cluster method, a method that is standardly used in quantum chemistry for highly accurate calculations. Coupled Cluster (CC) is normally formulated as an ansatz for the approximation of the Galerkin solution of the Schrödinger equation with in a given discretisation [1]. We globalise this ansatz to infinite dimensional spaces, thus obtaining an equivalent reformulation of the original, continuous Schrödinger equation in terms of a root equation for a nonlinear operator corresponding in this setting to the finite dimensional CC function f. We show local strong monontonicity of the CC function, derive some existence and uniqueness results and prove a goal-oriented error estimator [2] for the ground state energy. We conclude with a short discussion of the algorithmic treatment of the CC root equation.

[1] R. Schneider, Num. Math. 113, 3, 2009.
[2] R. Becker, R. Rannacher, Acta Numerica 2000 (A. Iserles, ed.), Cambridge University Press, 2001
