

On a time-dependent Kohn-Sham equation and related optimal control problems

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A Kohn-Sham equation is a system of nonlinear coupled Schrödinger equations that describe multi-particle quantum systems in the framework of the time-dependent density functional theory.

In the first part of this talk, existence, uniqueness and regularity of solutions to a time-dependent Kohn-Sham equation are investigated. Further, in view of control applications, the presence of a control function and of an inhomogeneity are also considered.

The second part of this talk is devoted to application models in quantum physics and chemistry that require to control many-electron systems to achieve a desired target configuration. In particular, the theory and numerical solution of optimal control problems governed by a Kohn-Sham model are discussed considering different objectives and a bilinear control mechanism. Results of numerical experiments demonstrate the computational effectiveness of the proposed control framework.