

*A Large Nonlinear Eigenvalue problem in
Hartree-Fock Equations*

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This talk discussed numerical algorithms for solution of Hartree-Fock equations. We suggest an approach to solve these equations using Toeplitz matrixes and bases with regular finite elements. It allows to construct a numerical algorithm with $N \log_2 N$ arithmetical complexity for the solution of large nonlinear eigenvalues problem, where N is a number of unknowns.

This approach is implemented in a program which allows to solve problems with up to million unknowns on a workstation for a reasonable time. The achieved results for predicting chemical data agree with the theory perfectly.