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REDUCED RANK EXTRAPOLATION APPLIED TO ELECTRONIC STRUCTURE COMPUTATIONS*

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Abstract. This paper presents a new approach for accelerating the convergence of a method for solving a nonlinear eigenvalue problem that arises in electronic structure computations. Specifically, we seek to solve the Schrödinger equation using the Kohn-Sham formulation. This requires the solution of a nonlinear eigenvalue problem. The currently prevailing method for determining an approximate solution is the Self-Consistent Field (SCF) method accelerated by Anderson's iterative procedure or a Broyden-type method. We propose to formulate the nonlinear eigenvalue problem as a nonlinear fixed point problem and to accelerate the convergence of fixed-point iteration by vector extrapolation. We revisit the reduced rank extrapolation method, a polynomial-type vector extrapolation method, and apply it in the RSDFT (real-space density functional theory) software.

Key words. nonlinear eigenvalue problem, vector extrapolation, Kohn-Sham equation, Anderson's method, Broyden's method, reduced rank extrapolation.

AMS subject classifications. 65H10, 65F10

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