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A Non-Linear Eigensolver-Based Alternative to Traditional Self-Consistent Electronic Structure Calculation Methods

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Abstract
This thesis presents a means of enhancing the iterative calculation techniques used in electronic structure calculations, particularly Kohn-Sham DFT. Based on the subspace iteration method of the FEAST eigenvalue solving algorithm, this nonlinear FEAST algorithm (NLFEAST) improves the convergence rate of traditional iterative methods and dramatically improves their robustness. A description of the algorithm is given, along with the results of numerical experiments that demonstrate its effectiveness and offer insight into the factors that determine how well it performs.

Advisor(s) or Committee Chair
Polizzi, Eric

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