A Nonlinear Eigensolver-Based Alternative to Traditional SCF Methods

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We present an iterative solution for nonlinear eigenvector problems (i.e. $H(\{\psi\})\psi = E\psi$) such as the one arising from the Kohn-Sham equations in density functional theory (DFT). The new strategy offers a very efficienct and robust alternative to the traditional self-consistent field (SCF) procedures used in electronic structure calculations (such as Newton-Broyden, Anderson mixing, direct inversion of the iterative subspace and mixed Pulay techniques). This is accomplished using a modification of the FEAST algorithm [1] applied to the full non-linear eigenvalue problem. From the complex contour integration of the projected Green's function, it is possible to obtain an approximate eigenvector subspace which is then used to derive a reduced non-linear eigenvector problem that is orders of magnitude smaller than the original one. The search subspace is then updated at each iteration of the FEAST algorithm until some quantity of interest (e.g. non-linear eigenvector residuals or total energy) converges (convergence is typically obtained in less than 10 iterations). The resulting approach is potentially one order of magnitude faster than conventional iterative methods, and it converges to the correct solution regardless of the choice of initial guess. Numerical examples are provided for various molecules (from H_2 to C_{60}) using Kohn-Sham/DFT/LDA and an all-electron finite element numerical framework in order to illustrate the robustness and efficiency of the new approach. A practical and straightforward 'black-box' implementation of the numerical strategy using the FEAST library package [2] will also be provided.

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[1] E. Polizzi, Phys. Rev. B **79**, 115112 (2009).

[2] http://www.ecs.umass.edu/∼polizzi/feast

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