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Robust Chebyshev-Filtered subspace iteration

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Chebyshev filtered subspace iteration (ChFSI) has been shown to be an effective solver for the eigenvalue problem embedded in self-consistent field iteration to solve the Kohn-Sham equations. However, a deficiency in ChFSI is that one it is sensitive to the choice of stopband $[a, b]$ lower endpoint a, and one must choose a filter degree d a priori. Poor choices will result in slower convergence or worse still, divergence. We present a robust version of Chebyshev filtered subspace iteration that recovers from too-small filter degrees d or too-small endpoints a. We introduce a heuristic to choose a d that is not too large. We also show that one can use byproducts of the Gram-Schmidt orthonormalization algorithm — a necessary part of ChFSI, to measure the effectiveness of the filter in removing unwanted eigenvectors. This allows one to simply continuing filtering until the angle between the new basis vector and unwanted eigenvectors is close enough to $\pi/2$, and to estimate when a is too small. Examples suggest that the run times and number of outer self-consistent field iterations are at least as small as the best d for standard ChFSI. We also show a test case for which our Robust Chebyshev Filtering recovers poor choice of a; ordinary ChFSI fails to converge for the same test case.