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Partial Rayleigh-Ritz procedure for quasi-minimal basis sets VINCENT MICHAUD-RIOUX, HONG GUO, McGill University — Recent Kohn-Sham DFT solver implementations [1-3] concentrate on building a subspace spanned by the occupied Kohn-Sham orbitals via Chebyshev filtering [1]. The Rayleigh-Ritz procedure is generally performed to populate the Kohn-Sham orbitals correctly and constitutes a major bottleneck in large electronic structure simulations. We found that the full diagonalization of the projected Hamiltonian can be avoided; only the partly occupied subspace is necessary since the fully occupied subspace can be obtained from the orthogonal complement of the former. For quasi-minimal basis sets, the size of the eigenvalue problem can be reduced significantly at the cost of constructing an orthogonal complement. The method can also be used with non-minimal basis sets such as atomic orbitals by performing a second projection of the Kohn-Sham Hamiltonian. The partial Rayleigh-Ritz procedure was implemented in our real space electronic structure calculator, which we used to conduct a performance comparison of the state-of-the-art Rayleigh-Ritz procedure against the partial Rayleigh-Ritz procedure. [1] Zhou, et al., Phys. Rev. E 74, 066704 (2006). [2] Motamarri, et al., Journal of Computational Physics 253, 308 (2013). [3] Levitt, A. and Torrent, M., Computer Physics Communications, In Press (2014)

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