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Precise all-electron response functions from a combined spectral sum and Sternheimer approach: application to EXX-OEP MARKUS BETZINGER, CHRISTOPH FRIEDRICH, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — The optimized-effective-potential (OEP) method is used to construct local potentials from non-local, orbital-dependent functionals, e.g., exact exchange (EXX). The method involves two response functions, which have to be converged to very high precision to obtain smooth and stable local potentials. Usually, this requires an exceptionally large orbital basis, leading to very costly calculations, especially for all-electron methods such as FLAPW [1]. In this work, we propose a scheme that combines the usual spectral sum from standard perturbation theory with a radial Sternheimer approach. It also comprises a, albeit small, Pulay-type correction, which refines the results especially for small basis sets. We demonstrate that with this new approach already the conventional minimal LAPW basis set is sufficient to yield precise response functions. Furthermore, very few unoccupied states are required, which reduces the computational cost considerably. The numerically important Sternheimer contribution arises from the potential dependence of the LAPW basis functions and is constructed by solving inexpensive radial differential equations. We show results for complex transition-metal oxides.

[1] M. Betzinger *et al.*, Phys. Rev. B **83**, 045105 (2011)

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