

## Improved method for generating exchange-correlation potentials from electronic wave functions

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Ryabinkin, Kohut, and Staroverov<sup>1</sup> devised an iterative method for reducing many-electron wave functions to Kohn–Sham exchange-correlation potentials. The original procedure works very well for large basis sets but sometimes fails for commonly-used small or medium basis sets. We present a modification<sup>2</sup> of the method’s working equation that makes the original procedure robust for all Gaussian basis sets and increases the accuracy of the resulting exchange-correlation potentials with respect to the basis-set limit. We also show that our modified procedure is capable of generating potentials for single-orbital Kohn-Sham systems in a single step, without performing iterations. Our potentials are free from oscillations that appear in exchange-correlation potentials obtained by Kohn-Sham inversion methods in finite Gaussian basis sets.

[1] I. G. Ryabinkin, S. V. Kohut, and V. N. Staroverov, *Phys. Rev. Lett.* **115**, 083001 (2015).

[2] E. Ospadov, I. G. Ryabinkin, and V. N. Staroverov, *J. Chem. Phys.* **146**, 084103 (2017).