Guaranteed convergence of a regularized Kohn-Sham iteration in finite dimensions

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The iterative Kohn-Sham scheme [1] has to date not been rigorously shown to converge to the correct ground-state density. This talk addresses the recent result of Penz *et al.* [2] that demonstrates the convergence of the exact Moreau-Yosida regularized theory in a finite-dimensional setting. This builds on previous work [3], where a similar iterative scheme was proposed that proved a weak type of convergence following an idea by Wagner *et al.* [4,5]. To obtain the desired convergence in both densities and potentials, the Moreau-Yosida regularization is key for the convergence proof in [2]. The regularization ensures differentiability of the universal Lieb functional [6] and was introduced in density-functional theory (DFT) by Kvaal *et al.* [7]. It has also recently been successfully applied to paramagnetic current DFT [8].

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