Energy expressions for model exchange potentials: Beyond the Levy–Perdew virial relation ALEX P. GAIDUK, VIKTOR N. STAROVEROV, University of Western Ontario — The common way to assign energies to Kohn–Sham exchange potentials is by using the Levy–Perdew virial relation. However, for model potentials that are not functional derivatives, this approach leads to energy expressions that lack translational invariance. We point out that there is a more general procedure for constructing density functionals from model potentials, of which the Levy–Perdew relation is just a special case. Using this generalization we propose a method for converting model potentials into density functionals that ensures translational invariance of the energy. To illustrate our approach we construct a competitively accurate exchange functional from the model potential of van Leeuwen and Baerends.

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