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**Ensemble density-functional theory for excited states: exact results versus approximations**[1] ZENGHUI YANG, University of Missouri - Columbia, AURORA PRIBRAM-JONES, KIERON BURKE, University of California - Irvine, RICHARD NEEDS, University of Cambridge, CARSTEN ULLRICH, University of Missouri - Columbia — The ensemble density-functional theory is an exact excited-state theory, but it is not used much in practice due to unsatisfactory approximated ensemble functionals. Unlike in ground-state density-functional theory, few exact conditions are known for the ensemble; because of this, the development of approximate functionals has been slow. We present a method for inverting the ensemble density to obtain the corresponding ensemble Kohn-Sham potential, and we illustrate it for highly accurate quantum Monte-Carlo densities of the helium atom. The resulting exact ensemble Kohn-Sham potential of helium shows prominent features that do not exist in known approximate ensemble functionals. In particular, the first excitation energy calculated from the exact ensemble is demonstrated to be invariant with respect to the mixing parameter of the ensemble. No known approximation has this exact property.

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