

Exchange-correlation potentials from many-electron wave functions

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We present a method for extracting the Kohn-Sham exchange-correlation potential from a given many-electron wave function. The potentials generated using our approach tend to the exact exchange-correlation potentials with increasing size of the basis set and the level of theory. We compute exchange-correlation potentials for several atoms and molecules and identify features in those potential that represent dynamic and nondynamic correlation effects included in the wavefunction description of the system.