Density-on-wave-function mapping beyond the Hohenberg-Kohn theorem

KLAUS CAPELLE, Federal University of ABC (UFABC) — Density-functional theory is based on the Hohenberg-Kohn theorem, establishing a one-to-one mapping between ground-state densities and wave functions. That theorem does not, however, make a direct statement on whether two wave functions that are in some sense close are mapped on two densities that are also close, and vice versa. In this work, a metric is defined that allows to quantify the meaning of “close” in the preceding sentence. This metric stratifies Hilbert space into concentric spheres on which maximum and minimum distances between states can be defined and geometrically interpreted. Numerical calculations for the Helium atom, Hooke’s atom and a lattice Hamiltonian show that the mapping between densities and ground states, which is highly complex and nonlocal in the coordinate description, in metric space becomes a monotonic and nearly linear mapping of vicinities onto vicinities. In this sense, the density-on-wave-function mapping is not only simpler than expected; it is as simple as it could be.