

Relating fundamentals of functional theory: An analytic case study

We provide a fully analytic analysis of fundamental aspects of reduced density matrix functional theory (RDMFT) for the generalized Hubbard dimer. For any generic reflection symmetric pair interaction, we derive the universal pure and ensemble functional with respect to both the real- and complex-valued Hilbert space. While the pure real functional is never convex, the remaining three functionals are always identical and follow as the lower convex envelope of the former. The underlying v -representability problem is solved analytically and the dependence of its solution on the pair interaction is highlighted.

Intriguingly, the gradient of each universal functional exhibits a square root dependent divergence at the boundary of the set of N -representable 1RDMs. The pair interaction affects only the prefactor of this distinctive behaviour. In that sense, this key finding emphasizes the universal character of the “fermionic exchange force”, recently found and proven in the context of translationally-invariant one-band lattice models.