

# Relating the pure and ensemble density matrix functional

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A crucial theorem in Reduced Density Matrix Functional Theory (RDMFT) suggested that the universal pure and ensemble functionals would coincide on their common domain of pure  $N$ -representable one-matrices. We refute this by a comprehensive analysis of the geometric picture underlying Levy's constrained search. Moreover, we then show that the ensemble functional follows instead as the lower convex envelop of the pure functional. It is particularly remarkable that the pure functional determines the ensemble functional even outside its own domain of pure  $N$ -representable one-matrices. From a general perspective, this demonstrates that relaxing pure RDMFT to ensemble RDMFT does not necessarily circumvent the complexity of the generalized Pauli constraints. Instead, the complexity may simply be transferred from the underlying space of pure  $N$ -representable one-matrices to the structure of the universal one-matrix functional.