Exact Excited-State Functionals of the Asymmetric Hubbard Dimer

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The exact functionals associated with the (singlet) ground and the two singlet excited states of the asymmetric Hubbard dimer at half-filling are calculated using both Levy’s constrained search and Lieb’s convex formulation. While the ground-state functional is, as commonly known, a convex function with respect to the density (or, more precisely, the site occupation), the functional associated with the (highest) doubly-excited state is found to be concave. Also, we find that, because the density of the first excited state is non-invertible, its “functional” is a partial, multi-valued function composed of one concave and one convex branch that correspond to two separate sets of values of the external potential. Remarkably, it is found that, although the one-to-one mapping between density and external potential may not apply (as in the case of the first excited state), each state-specific energy and corresponding universal functional are “functions” whose derivatives are each other’s inverse, just as in the ground state formalism.



Figure 1. State-specific exact functionals Fn(ρ) as functions of ρ for t=1/2 and U = 1.