

Reduced Density-Matrix Functional Theory: correlation and spectroscopy

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In this work we explore the performance of approximations to electron correlation in reduced density-matrix functional theory (RDMFT) [1] and of approximations to the observables calculated within this theory. Our analysis focuses on the calculation of total energies, occupation numbers, removal/addition energies, and spectral functions. We use the exactly solvable Hubbard molecule at 1/4 and 1/2 filling as test systems. This allows us to analyze the underlying physics and to elucidate the origin of the observed trends. For comparison we also report the results of the *GW* approximation, where the self-energy functional is approximated, but no further hypothesis are made concerning the approximations of the observables. In particular we focus on the atomic limit, where the two sites of the molecule are pulled apart and electrons localize on either site with equal probability, unless a small perturbation is present: this is the regime of strong electron correlation. In this limit, using the Hubbard molecule at 1/2 filling with or without a spin-symmetry-broken ground state, allows us to explore how degeneracies and spin-symmetry breaking are treated in RDMFT. We find that, within the used approximations, neither in RDMFT nor in *GW* the signature of strong correlation are present in the spin-singlet ground state, whereas both give the exact result for the spin-symmetry broken case. Moreover we show how the spectroscopic properties change from one spin structure to the other. Our findings can be generalized to other situations, which allows us to make connections to real materials and experiment. [2]

[1] T. L. Gilbert, Phys. Rev. B 12, 2111 (1975)

[2] S. Di Sabatino, J.A. Berger, L. Reining, and P. Romaniello, arXiv:1409.1008