

Abstract Submitted
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Bridging density-functional and many-body perturbation theory: orbital-density dependence in electronic-structure functionals ANDREA FERRETTI, S3 Center, CNR - Istituto Nanoscienze, Modena, Italy., ISMAILA DABO, CERMICS, Université Paris-Est, MATTEO COCOCCIONI, CEMS, University of Minnesota, NICOLA MARZARI, Department of Materials, Oxford University — Energy functionals which depend explicitly on the orbital densities (ODD), instead of the total charge density, appear when applying self-interaction corrections to density-functional theory. In these cases (e.g. the Perdew-Zunger [1] and the non-Koopmans [2] approaches) the total energy loses invariance under unitary rotations of the orbitals, and the minimization of the functionals leads to orbital-dependent Hamiltonians. We show that it is possible to identify the orbital-dependency of densities and potentials with an effective and discretized frequency-dependency, in close analogy to the quasi-particle approximation of frequency-dependent self-energies and naturally oriented to interpret electronic spectroscopies [3]. Some of the existing ODD functionals are analyzed from this new perspective. Numerical results for the electronic structure of gas-phase molecules (within the Koopmans-corrected class of functionals) are computed and found in excellent agreement with photoemission (UPS) data. [1] J.-P. Perdew and A. Zunger, *Phys. Rev. B* 23, 5048 (1981). [2] I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, M. Cococcioni, *Phys. Rev. B* 82, 115121 (2010). [3] M. Gatti, V. Olevano, L. Reining, I.-V. Tokatly, *Phys. Rev. Lett.* 99, 057401 (2007).

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