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Spectral function from Reduced Density Matrix Functional Theory PINA ROMANIELLO, STEFANO DI SABATINO, LPT, CNRS, IRSAMC, University Toulouse III - Paul Sabatier, France and European Theoretical Spectroscopy Facility, JAN A. BERGER, LCPQ, IRSAMC, University Toulouse III - Paul Sabatier, CNRS, France and European Theoretical Spectroscopy Facility, LUCIA REINING, LSI, Ecole Polytechnique, CNRS, CEA-DSM, France and European Theoretical Spectroscopy Facility — In this work we focus on the calculation of the spectral function, which determines, for example, photoemission spectra, from reduced density matrix functional theory. Starting from its definition in terms of the one-body Green's function we derive an expression for the spectral function that depends on the natural occupation numbers and on an effective energy [1] which accounts for all the charged excitations. This effective energy depends on the two-body as well as higher-order density matrices. Various approximations to this expression are explored by using the exactly solvable Hubbard chains [2].

[1] J.A. Berger, L. Reining, and F. Sottile, Phys. Rev. B 82, 041103 (2010)
[2] S. Di Sabatino, J.A. Berger, L. Reining, and P. Romaniello, in preparation

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