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Reduced Density-Matrix Functional Theory: correlation and spectroscopy STEFANO DI SABATINO, Laboratoire de Physique Théorique, CNRS, IRSAMC, Université Paul Sabatier, Toulouse, France and European Theoretical Spectroscopy Facility, ARJAN BERGER, Laboratoire de Chimie et Physique Quantiques, IRSAMC, Universite Paul Sabatier, CNRS, Toulouse, France and European Theoretical Spectroscopy Facility, LUCIA REINING, Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, Palaiseau, France and European Theoretical Spectroscopy Facility, PINA ROMANIELLO, Laboratoire de Physique Théorique, CNRS, IRSAMC, Université Paul Sabatier, Toulouse, France and European Theoretical Spectroscopy Facility — In this work we explore the performance of approximations to electron correlation in reduced density-matrix functional theory (RDMFT) and of approximations to the observables calculated within this theory[1]. Particular focus is put on the spectral function, which determines, for example, photoemission spectra, and which cannot be obtained in a straightforward way from the density matrix, and on the regime of strong electron correlation, which is difficult to treat by standard methods. Using the simple Hubbard model as test case shines light on the content, successes and limits of current RDMFT approaches.

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