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On the formulation of a density matrix functional for Van der Waals interaction of like- and opposite-spin electrons in the helium dimer

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Abstract

Whereas a density functional that incorporates dispersion interaction has remained elusive to date, we demonstrate that in principle the dispersion energy can be obtained from a density matrix functional. In density matrix functional theory one tries to find suitable approximations to the two-particle reduced density matrix (2RDM) in terms of natural orbitals (NOs) and natural orbital occupation numbers (ONs). The total energy is then given as a function(al) of the NOs and ONs, i.e., as an implicit functional of the 1RDM. The left-right correlation in a (dissociating) bond, as well as various types of dynamical correlation, can be described accurately with a NO functional employing only J and K integrals (JK-only functional). We give a detailed analysis of the full CI wavefunction of the He-2 dimer, from which the dispersion part of the two-particle density matrix is obtained. It emerges that the entirely different physics embodied in the dispersion interaction leads to an essentially different type of exchange-correlation orbital functional for the dispersion energy (non-JK). The distinct NO functionals for the different types of correlation imply that they can be used in conjunction without problems of double counting. Requirements on the (primitive) basis set for Van der Waals bonding appear to be more modest than for other types of correlation. (C) 2012 American Institute of Physics.

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