TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY FOR STRONGLY INTERACTING ELECTRONS

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We consider an analytically solvable model of two interacting electrons that allows for the calculation of the exact exchange-correlation kernel of time-dependent density functional theory. This kernel as well as the corresponding density response function is studied in the limit of large repulsive interactions between the electrons and we give analytical results for these quantities as an asymptotic expansion in powers of the square root of the interaction strength. We find that, depending on the symmetry of an applied perturbation, the induced density changes are either suppressed at strong interaction strengths or else involve the excitation of modes that are independent of the interaction strength and in the model can be related to doubly excited states. We further derive an alternative asymptotic series for the kernel in the strong interaction limit on the basis of the theory developed in [1] using the formalism of strictly correlated electrons in the adiabatic approximation. We find that the first two leading terms in this series, which physically correspond to the strictly correlated limit and the zero-point vibrations around it, coincide with the two leading terms of the exact expansion and give a physical interpretation of this fact. The ability to reproduce exact quantities in the strong interaction limit establishes the usefulness of the strictly correlated electron formalism to study the density response and excitation properties for systems with strong electron interactions.

[1] Lani, G, di Marino, S, Gerolin, A, van Leeuwen, R and Gori-Giorgi, P, *Phys. Chem. Chem. Phys.*, **2016**, 18, 21092-21101