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Correlation Energy of the Homogeneous Electron Gas from Adiabatic Connection Fluctuation-Dissipation Theory including Exact Exchange kernel NICOLA COLONNA, STEFANO DE GIRONCOLI, SISSA - International School for Advanced Studies — We have developed an expression for the electronic correlation energy via the Adiabatic Connection Fluctuation-Dissipation Theorem (ACFDT) going beyond the Random-Phase Approximation (RPA) by including exact exchange contribution to the kernel (RPAx). Our derivation is valid and efficient for general systems. It is based on an eigenvalue decomposition of the time dependent response function of the Many Body system in the limit of vanishing coupling constant, evaluated by Density Functional Perturbation Theory. We tested the accuracy of this approximation on the homogeneous electron gas. Within RPAx, the correlation energy of the homogeneous electron gas improves significantly with respect to the RPA results up to densities of the order of $r_s \approx 10$. However, beyond this value, the RPAx response function becomes pathological and the approximation breaks down. We have also evaluated the dependence of the correlation energy on the spin magnetization of the system. Both RPA an RPAx are in excellent agreement with accurate Quantum Monte Carlo results.

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