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Exchange-correlation functionals from a local interpolation along the adiabatic connection STEFAN VUCKOVIC, VU University Amsterdam, TOM IRONS, ANDREW TEALE, Nottingham University, ANDREAS SAVIN, UMPC Paris, PAOLA GORI-GIORGI, VU University Amsterdam — We use the adiabatic connection formalism to construct a density functional by doing an interpolation between the weak and the strong coupling regime. Combining the information from the two limits, we are able to construct an exchange-correlation (xc) density functional free of the bias towards weakly correlated system, which is present in the majority of approximate xc functionals. Previous attempts in doing the interpolation between the two regimes, such as the interaction strength interpolation (ISI), had a fundamental flaw: the lack of size-consistency, as the corresponding functional depends non-linearly on the global (integrated over all space) ingredients. To recover size-consistency in such a framework, we move from the global to local quantities. We use the energy densities as local quantities in the gauge of the electrostatic potential of the xc hole. We use the "strictly-correlated electrons" (SCE) approach to compute the energy densities in the strong-coupling limit and the Lieb maximization algorithm to extract the energy densities from the low-coupling regime. We then test the accuracy of the local interpolation schemes by using the nearly exact local energy densities. In this talk I am going to present our results with the emphasis on strongly correlated systems.

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