Adiabatic-connection fluctuation-dissipation DFT for the structural properties of solids - the renormalized ALDA and other electron gas kernels

CHRISTOPHER PATRICK, KRISTIAN THYGESEN, Department of Physics, Technical University of Denmark — The adiabatic-connection fluctuation-dissipation formulation of density-functional theory (ACFD-DFT) provides a natural pathway for the calculation of electron correlation energies going beyond the random-phase approximation (RPA). The key ingredient of ACFD-DFT is the exchange-correlation kernel $f_{xc}$ of time-dependent DFT. The last few decades have seen the development of a number of model kernels, often based on studies of the homogeneous electron gas (HEG). Here, we introduce a selection of these HEG kernels and use them to calculate the structural properties of a test set of solids within ACFD-DFT. Amongst our kernels we include the recently-introduced renormalized adiabatic local-density approximation (rALDA) [T. Olsen and K. S. Thygesen, Phys. Rev. B 88, 115131 (2013)], and also consider kernels which (a) satisfy known limits of the HEG, (b) carry a frequency dependence or (c) include a long-range component. By comparing the kernels to each other, to the RPA and to experiment we shall identify the essential properties of a kernel for ACFD-DFT applications. We shall also discuss the technical challenges of applying HEG kernels to inhomogenous systems, and identify key areas for future progress.

1Research supported by the Danish Council for Independent Research’s Sapere Aude Program, Grant No. 11-1051390