Two-Point Nonlocal Density Functionals for the Kinetic Energy and Exchange-Correlation Energy

Paul W. Ayers

Department of Chemistry & Chemical Biology; McMaster University; Canada

Many of the problems in density-functional theory can be mitigated by carefully designing an exchange-correlation hole with the proper mathematical properties. This leads to generalized and extended versions of the venerable weighted density approximation (WDA). In this talk, I will show how well WDA can work for the kinetic energy, exchange energy, and exchange-correlation energy. One advantageous feature of the WDA is that it allows one to deal with fractionally occupied sites in a better way than conventional functionals.The traditional criticism of WDA has been its high computational cost. These costs are mitigated by new algorithms (a) using a new limited-memory quasi-Newton method that was designed especially for this application and (b) expanding integrands in explicitly-correlated basis sets, obviating the need for numerical integration.