

An efficient non-pairwise-additive correlation energy functional for dispersion forces

John F. Dobson and Tim Gould

We use the continuum mechanics (CM) of Tao, Gao, Tokatly and Vignale [PRL **81**, 195106 (2010)] to describe electronic response of inhomogeneous electronic systems to effective fields. We thereby obtain an approximation to the RPA correlation energy that is computationally efficient and describes long-ranged (e.g. van der Waals) correlations beyond the pairwise-additive approximation. So far this approach has been tested successfully on the case of two thin parallel metal slabs at all separations D down to overlap of the electronic clouds [ArXiv:1106.0327v2]. Our method reproduced full (d)RPA results well for all D values, and gave the correct asymptote $E = -CD^{-5/2}$ at large separations $D \rightarrow \infty$, in contrast to the present generation of efficient van der Waals functionals. The CM theory also gives the exact response of quantal one-electron systems. Development of the method for periodic systems is underway.