Ramifications of the Optimized Effective Potential of Jim Talman

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One of the most pervasive contributions of Jim Talman has been the formulation and development of the optimized effective potential (OEP) that can be viewed as a way to tie density functional theory (DFT) and ab initio wave function theory (WFT) together. The original work was for the exchange potential in DFT, but the concept is equally good for electron correlation subject to a different way of imposing the condition. We call that the 'density condition' which insists that the Vxc obtained be uniquely defined from a known, orbital dependent expression such that the Kohn-Sham determinant will provide the correct, correlated density once the orbitals are determined self-consistently. This is the foundation for what we call ab initio DFT as unlike any other DFT realization, this procedure has to lead to the exact answer in the basis set and correlation limit like in WFT. But since the potential is local, they can be plotted to see how they differ from the forms normally used. Some ramifications of this OE procedure are discussed and used to provide better DFT results.

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