A.2.3   Passage to natural basis

The passage in the natural basis at this stage is not part of the scheme of the annals of physics, article. But it is very convenient from a programming perspective to have directly the natural basis, and the corresponding occupation numbers to store them for further use in the correction of Energy. An alternative is to compute separately the total occupation numbers per spin, without diagonalizing the norm matrix. This second alternative has also been implemented, and produces almost identical results. The passage to natural basis is done with the method described in the current projected article. The resulting wave functions and occupation numbers are stored as φ^{orth} and W_α^{orth} for further use. Then the density, fields and energy are computed, and the Kohn Sham energy is stored as EKS^{ref}. We also store the total occupation for each spin, and the total single particle energy per spin, for further use in the energy correction, as it is important to conserve the total occupation per spin.

A.2.4   Computation of DCMF state

Overview

Lets first define some notations:

- φ_α^{orth} the wave functions after passage in the natural basis

- W_α^{orth} the corresponding occupation numbers

- ρ_0 the corresponding density: $\rho_0(\mathbf{r}, t) = \sum_\alpha W_\alpha^{orth} \varphi_\alpha^{orth}(\mathbf{r}, t)$