hartree-fock

Amanda Dumi

July 19, 2018

background

slater determinant

We need a wavefunction consisting of:

- orthogonal wavefunctions of individual particles
- follow antisymmetry requirement

$$\Phi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \chi_1(x_1) & \chi_2(x_1) & \cdots & \chi_N(x_1) \\ \chi_1(x_2) & \chi_2(x_2) & \cdots & \chi_N(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \chi_1(x_N) & \chi_2(x_N) & \cdots & \chi_N(x_N) \end{vmatrix}$$

realm of methods

Exact answer:

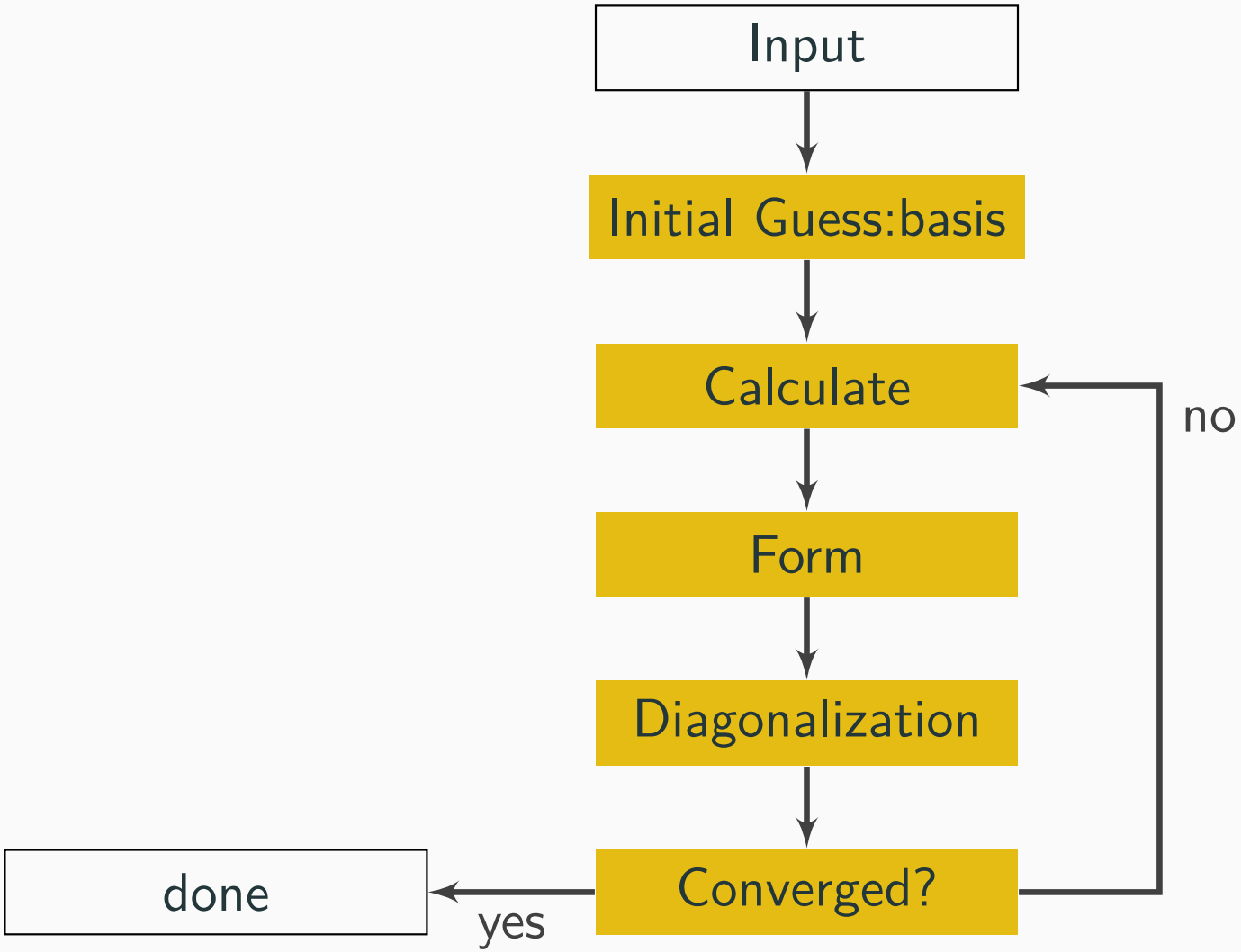
$$\Psi = \sum_{K}^{\infty} D_k \Phi_K$$

Hartree-Fock instead uses a single slater determinant for the ground state

$$\Psi = \Phi_0$$

All effort goes towards finding the best set of orbitals.

self consistent field



algorithm

derivation

example

background

can we improve?

missing correlation energy

correlation energy