Computational Materials Physics

Center for Molecular Modeling

Department of Materials Science and Engineering

(post-)Hartree-Fock method(s)

Stefaan.Cottenier@ugent.be
Technologiepark 903, Zwijnaarde

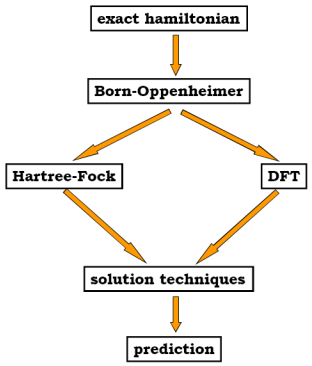
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

three levels of approximations

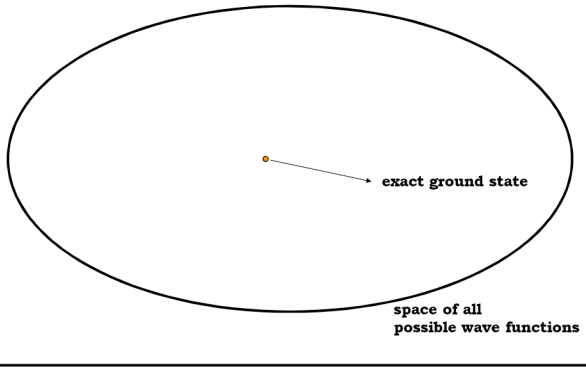
level 1:

level 2:

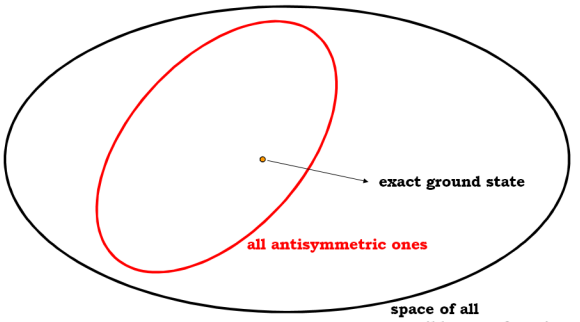
level 3:



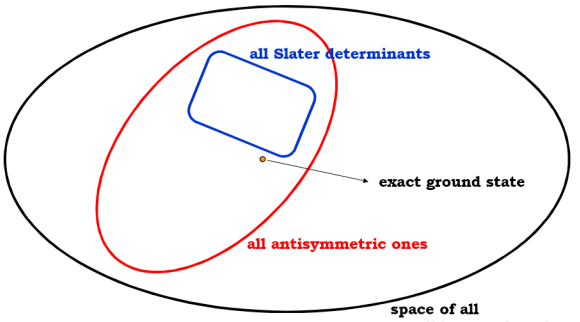
(post-)Hartree-Fock methods



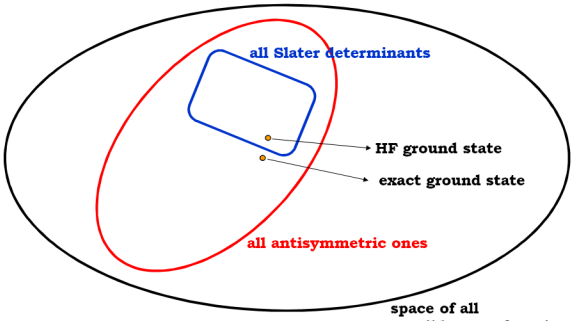
(post-)Hartree-Fock methods



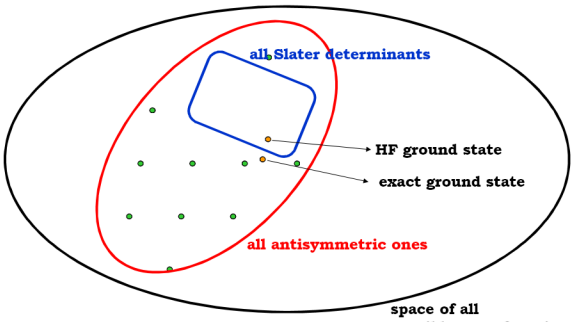
(post-)Hartree-Fock methods



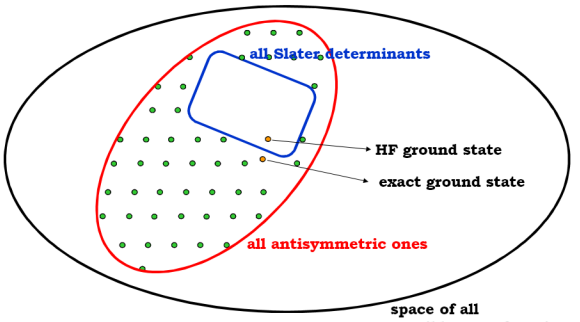
(post-)Hartree-Fock methods



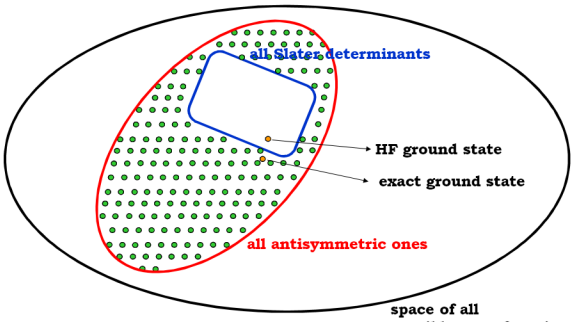
(post-)Hartree-Fock methods



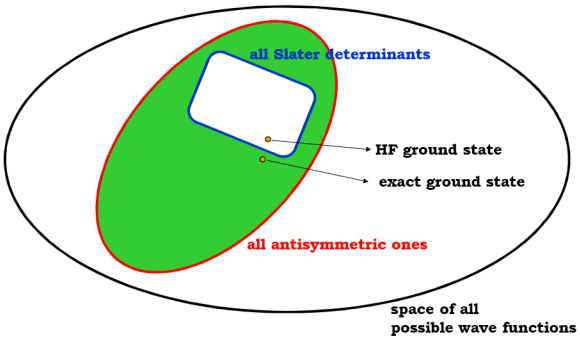
(post-)Hartree-Fock methods



(post-)Hartree-Fock methods



(post-)Hartree-Fock methods



(post-)Hartree-Fock methods

The HF method as such is not very accurate for solids, and is therefore not really used. But it forms the starting point for **post-Hartree-Fock methods** that are routinely used:

- coupled cluster theory (CCSD(T))
- Mølller-Plesset perturbation theory (MP2)
- configuration interaction (CI)
- CASSCF
- MRCI
- ...

➔ typical topics in a quantum chemistry course.