Project - FYS4411

Henrik Andersen Sveinsson

February 7, 2014

Abstract

1 The Hartree-Fock method

1.1 Approximations

There are five main approximations in the Hartree-Fock method:

- The Born-Oppenheimer approximation
- Relativistic effects are neglected
- The solution is a linear combination of (typically orthogonal) basis functions
- Each energy eigenfunction is assumed to be describable by a single Slater determinant
- The mean field approximation is implied.

The Hartree equation in atomic units:

$$\left[-\frac{1}{2}\nabla^2 - \sum_n \frac{Z_n}{|\mathbf{r}-\mathbf{R}_n|} + \sum_{l=1}^{N} \int \mathrm{d}x' |\psi_l(\mathbf{x})|^2 \frac{1}{|\mathbf{r}-\mathbf{r}'|}\right] \psi_k(\mathbf{x}) = E'\psi_k(\mathbf{x}) \quad (1)$$

Note that $\mathbf{x}' = (\mathbf{r}', s')$, so that $\int \mathrm{d}x' = \sum_{s'} \int \mathrm{d}\mathbf{r}'$.