Report on hartree fock

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1 Introduction

In this report a brief overview will be given of how the Hartree Fock theory is developed and what it is used for in solving the energy of a molecular system.

2 Born-Oppenheimer approximation

2.1 The molecular Hamiltonian

$$\begin{aligned}\hat{H} =& \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m_e}\nabla_i^2 + \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\j\neq i}}^{N}\frac{e^2}{4\pi\epsilon_0|\mathbf{r}_i-\mathbf{r}_j|}\right)\\ &+\sum_{A=1}^{M}\left(-\frac{\hbar^2}{2M_A}\nabla_A^2 + \frac{1}{2}\sum_{A=1}^{M}\sum_{\substack{B=1\\B\neq A}}^{M}\frac{Z_A Z_B e^2}{4\pi\epsilon_0|\mathbf{R}_A-\mathbf{R}_B|}\right)\\ &-\sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A e^2}{4\pi\epsilon_0|\mathbf{r}_i-\mathbf{R}_A|}\end{aligned} \tag{2.1}$$