PHYS 3317: Hartree

Hand in at beginning of next lecture

Because of Fermionic statistics, we know that no two electron can be in the same state. A variational model of this is the “Hartree” model,

$$\psi(r_1, r_2, \cdots, r_n) = \phi_1(r_1)\phi_2(r_2)\cdots\phi_n(r_n), \tag{1}$$

where

$$\int dr\, \phi_i^*(r)\phi_j(r) = \delta_{ij}. \tag{2}$$

This neglects spins, which are easy enough to add later. It also does not fully account for Fermionic statistics. The simplest way to incorporate these statistics yields the ”Hartree-Fock model”, which we will discuss separately.

Problem 1. Show that

$$\int dr_1\, dr_2 \cdots dr_n\, \psi^*(r_1, r_2, \cdots, r_n)\psi(r_1, r_2, \cdots, r_n) = 1 \tag{3}$$

Solution 1.1.

Problem 2. Write

$$T_1 = \int dr_1\, dr_2 \cdots dr_n\, \psi^*(r_1, r_2, \cdots, r_n) \left(-\frac{\hbar^2}{2m}\nabla_1^2\right) \psi(r_1, r_2, \cdots, r_n) \tag{4}$$

in terms of an integral involving only ϕ_1.

Solution 2.1.

Problem 3. For any single particle potential $V(r)$, write

$$V_1 = \int dr_1\, dr_2 \cdots dr_n\, \psi^*(r_1, r_2, \cdots, r_n) V(r_1) \psi(r_1, r_2, \cdots, r_n) \tag{5}$$

in terms of an integral involving only ϕ_1.

Solution 3.1.

Problem 4. For any pairwise potential $U(r_1 - r_2)$, write

$$U_{12} = \int dr_1\, dr_2 \cdots dr_n\, \psi^*(r_1, r_2, \cdots, r_n) U(r_1 - r_2) \psi(r_1, r_2, \cdots, r_n) \tag{6}$$

in terms of an integral involving only ϕ_1 and ϕ_2.

Solution 4.1.

Problem 5. The Hamiltonian for the electrons in an atom is

$$H = \sum_j \left[-\frac{\hbar^2}{2m} \nabla_j^2 - \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{r_j} \right] + \sum_{i<j} \frac{e^2}{4\pi\epsilon_0} \frac{1}{|r_i - r_j|}. \tag{7}$$

Express $\langle H \rangle$ as a sum of integrals over the wavefunctions ϕ_j.

Solution 5.1.