



## 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,

$$\psi(r_1, r_2, \dots, r_n) = \phi_1(r_1)\phi_2(r_2) \cdots \phi_n(r_n), \quad (1)$$

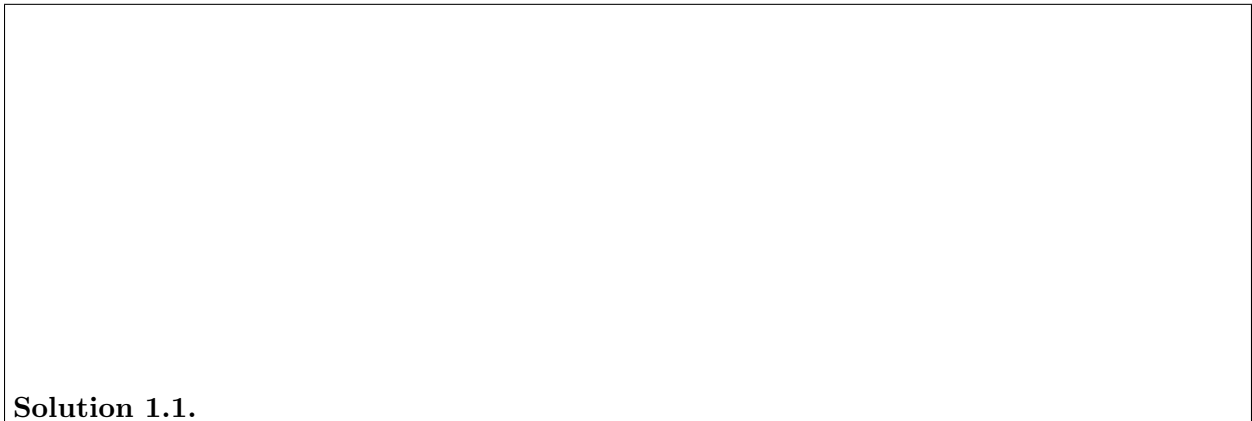
where

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

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

$$\int dr_1 dr_2 \cdots dr_n \psi^*(r_1, r_2, \dots, r_n)\psi(r_1, r_2, \dots, r_n) = 1 \quad (3)$$



**Solution 1.1.**



**Problem 2.** Write

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

in terms of an integral involving only  $\phi_1$ .

**Solution 2.1.**

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

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

in terms of an integral involving only  $\phi_1$ .

**Solution 3.1.**

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

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

in terms of an integral involving only  $\phi_1$  and  $\phi_2$ .

**Solution 4.1.**

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

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

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

**Solution 5.1.**