

Physics 4410
Quantum Mechanics 2

Lecture 23

The Hartree-Fock approximation

October 21, 2020

1. Consider the Hamiltonian

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(x_1) + V(x_2) + U(x_1, x_2).$$

Describe the Hartree-Fock trial wave function for fermions (ignore spin).

2. What is $\langle H \rangle$?

3. Use variational calculus (Euler-Lagrange!) to choose the optimal wave functions. Interpret the result.

4. Summarize/generalize the Hartree-Fock approximation.

Activity: Atoms in the periodic table.

- (a) Predict the most stable atoms (i.e. those that have the largest gap between the ground state and first excited state) if we ignore electron-electron interactions.

(b) Sketch the s, p, and d orbitals of hydrogen. Which are farther from the nucleus (on average)?

(c) Explain the qualitative structure of the periodic table.