Homework #6. October 30

Topics:  second quantization (normal order and expectation values)
                     Wick’s theorem
                     Hartree-Fock equations

1. Use Wick’s theorem to transform the operator product \( A = a_j a_i^\dagger a_k^\dagger a_l^\dagger \) to normal form.

   Hint: use example given in the lecture to write out

   \[ A = :A:+ :A: \]

2. Use Wick’s theorem to calculate the expectation value \( \langle 0 | a_i a_j a_k a_l a_m a_n | 0 \rangle \).

3. Consider an atom with \( n \) electrons. The state \( |0_c\rangle \) represents the core with filled subshells:

   \[ |0_c\rangle = a_{a_1} a_{a_2} \ldots |0\rangle \].

   The following designations are accepted: letters in the beginning of the alphabet (\( a, b, c, d \)) designate core orbitals and letters \( m, n, r, s \) designate excited (and non-core) orbitals.

   Which of the following operator products are in normal form?

   \[ (a) \ a_{m} a_{a}^\dagger \quad (d) \ a_{m} a_{a}^\dagger a_{b}^\dagger a_{b} \]

   \[ (b) \ a_{a} a_{m}^\dagger \quad (e) \ a_{c} a_{d}^\dagger a_{a} a_{b} \]

   \[ (c) \ a_{a} a_{b}^\dagger \quad (f) \ a_{c} a_{b} a_{d}^\dagger a_{c} \]

   Calculate the expectation value of each of these products in the core state, i.e., \( \langle 0_c | A | 0_c \rangle \).

4. Write down in detail the Hartree-Fock equations for the 3 closed shells (1s, 2s, and 2p) of the neon atom. Hint: the equation for the 1s shell (in atomic units) is

   \[
   h_0 P_{1s} + V_{dir} P_{1s} - \left[ v_0(1s, r) P_{1s} + v_0(2s, 1s, r) P_{1s} + v_1(2p, 1s, r) P_{2p} \right] = e_{1s} P_{1s}
   \]

   where

   \[
   h_0 P_{nl} = \left( -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{Ze}{r} \right) P_{nl}
   \]

   \[
   V_{dir} = 2v_0(1s, r) + 2v_0(2s, r) + 6v_0(2p, r)
   \]

DUE: November 11