Quiz #3. November 11

Name

Grade? YES NO

Topics: second quantization
        expectation values
        Wick’s theorem
        Coulomb matrix elements
        HF equations

1. Apply Wick’s theorem to write the operator product \( a_k a_l a_i a_j \) as a sum of normal-ordered terms. Calculate the expectation values \( \langle 0 | a_k a_l a_i a_j | 0 \rangle \) and \( \langle 0 | a_i a_j a_k a_l | 0 \rangle \).

2. We define the “new vacuum” as \( |0_c \rangle = a_d a_{d'} ... a_{d'} |0 \rangle \), consisting of filled sub-shells (for example \( 1s^22s^22p^6 \) for neon). We designate filled sub-shell (core) orbitals \( a, b, ... \) and orbitals not in the core \( m, n, ... \). Which of the following is true?

\[
\begin{align*}
a_a |0_c \rangle &= 0 \\
a_m |0_c \rangle &= 0 \\
a_m |0_c \rangle &= 0 \\
a_a |0_c \rangle &= 0 \\
\left( a_m | a_a \right) &= 0 \\
\left( a_m | a_n \right) &= 0 \\
\left( a_m | a_n \right) &= 0
\end{align*}
\]

3. Write down the Hartree-Fock equation for the 1s orbital of He atom.

4. Write the expression for the Coulomb matrix element \( g_{abcd} \).

5. Derive the expression for the Coulomb matrix element \( g_{abcd} \).

6. Write down the Hartree-Fock equation for the 1s orbital of Be atom.