

4) Exercises

1) Verify the following commutation and anticommutation relations

a) $[\hat{A}, \hat{B}_1 \hat{B}_2] = [\hat{A}, \hat{B}_1] \hat{B}_2 + \hat{B}_1 [\hat{A}, \hat{B}_2]$

b) $[\hat{A}, \hat{B}_1 \hat{B}_2]_{+} = [\hat{A}, \hat{B}_1]_{+} \hat{B}_2 - \hat{B}_1 [\hat{A}, \hat{B}_2]_{+}$

c) $[\hat{A}, \hat{B}_1 \dots \hat{B}_n]_{+} = \sum_{k=1}^n (-1)^{k-1} \hat{B}_1 \dots \hat{B}_{k-1} [\hat{A}, \hat{B}_k]_{+} \dots \hat{B}_n$ (n odd)

2) Verify the following relations for matrix exponentials

a) $(\exp(A))^{\dagger} = \exp(A^{\dagger})$

b) $B \exp(A) B^{-1} = \exp(B A B^{-1})$

c) $\exp(A+B) = \exp(A) \exp(B)$ if $[A, B] = 0$

d) $\frac{d}{d\lambda} \exp(\lambda A) = A \exp(\lambda A) = \exp(\lambda A) A$

e) $\exp(-A) B \exp(A) = B + [B, A] + \frac{1}{2!} [[B, A], A] + \frac{1}{3!} [[[B, A], A], A] + \dots$

3) Prove the following commutation relations for excitation operators

$E_{pq} = a_p^{\dagger} a_q$ $[E_{pq}, E_{rs}] = \delta_{ps} E_{rq} - \delta_{rs} E_{pq}$

4) Prove that the MP2 energy expression

$$E^{MP2} = - \sum_{i < j} \sum_{a < b} \frac{|g_{aibj} - g_{ajbi}|^2}{\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j}$$

is size-extensive.

Hint: take two non-interacting systems and group occupied and virtual orbitals together on basis of their location in either the first or the second system.