

Física Atómica y Molecular

Tarea 02: Método de Hartree-Fock

Dr. Omar De la Peña Seaman

4 septiembre 2026

Nombre del Estudiante: _____

Problema 1 *Koopmans' theorem*

Demonstrate the Koopman's theorem,

$$E_{HF}(N-1) - E_{HF}(N) \approx -\epsilon_n,$$

$$E_{HF}(N+1) - E_{HF}(N) \approx \epsilon_m,$$

where we have assumed that an electron of the n th orbital has been removed, and that an extra electron has been added to the m th orbital. $E_{HF}(M)$ is the total electronic energy for the M -electron system.

.....