Exercises FYS4480, week 38, September 19-23, 2022

Exercise 1

a) Show that the onebody part of the Hamiltonian

$$\hat{H}_0 = \sum_{pq} \langle p|\hat{h}_0|q\rangle a_p^\dagger a_q$$

can be written, using standard annihilation and creation operators, in normal-ordered form as

$$\begin{aligned}\hat{H}_0 &= \sum_{pq} \langle p|\hat{h}_0|q\rangle a_p^\dagger a_q \\ &= \sum_{pq} \langle p|\hat{h}_0|q\rangle \left\{a_p^\dagger a_q\right\} + \delta_{pq\in i} \sum_{pq} \langle p|\hat{h}_0|q\rangle \\ &= \sum_{pq} \langle p|\hat{h}_0|q\rangle \left\{a_p^\dagger a_q\right\} + \sum_{i} \langle i|\hat{h}_0|i\rangle\end{aligned}$$

Explain the meaning of the various symbols. Which reference vacuum has been used?

b) Show that the twobody part of the Hamiltonian

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs} \langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

can be written, using standard annihilation and creation operators, in normal-ordered form as

$$\begin{aligned}\hat{H}_I &= \frac{1}{4}\sum_{pqrs} \langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r \\ &= \frac{1}{4}\sum_{pqrs} \langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \sum_{pqi} \langle pi|\hat{v}|qi\rangle \left\{a_p^\dagger a_q\right\} + \frac{1}{2}\sum_{ij} \langle ij|\hat{v}|ij\rangle\end{aligned}$$

Explain again the meaning of the various symbols. The two-body matrix elements are anti-symmetrized.

Exercise 2

Consider a Slater determinant built up of single-particle orbitals ψ_λ, with $\lambda = 1, 2, \ldots, N$.
The unitary transformation

$$\psi_a = \sum_\lambda C_{a\lambda}\phi_\lambda,$$

brings us into the new basis. The new basis has quantum numbers $a = 1, 2, \ldots, N$. Show that the new basis is orthonormal. Show that the new Slater determinant constructed from the new single-particle wave functions can be written as the determinant based on the previous basis and the determinant of the matrix C. Show that the old and the new Slater determinants are equal up to a complex constant with absolute value unity. (Hint, C is a unitary matrix).