

Exercises FYS4480, week 38, September 25-29, 2023

Exercise 1

We define the one-particle operator

$$\hat{T} = \sum_{\alpha\beta} \langle \alpha | t | \beta \rangle a_{\alpha}^{\dagger} a_{\beta},$$

and the two-particle operator

$$\hat{V} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}.$$

We have defined a single-particle basis with quantum numbers given by the set of greek letters $\alpha, \beta, \gamma, \dots$

- a) Show that the form of these operators remain unchanged under a transformation of the single-particle basis given by

$$|i\rangle = \sum_{\lambda} |\lambda\rangle \langle \lambda | i \rangle,$$

with $\lambda \in \{\alpha, \beta, \gamma, \dots\}$. Show also that $a_i^{\dagger} a_i$ is the number operator for the orbital $|i\rangle$.

- b) Find also the expressions for the operators T and V when T is diagonal in the representation i .

Exercise 2

Consider a Slater determinant built up of single-particle orbitals ψ_{λ} , with $\lambda = 1, 2, \dots, N$. The unitary transformation

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

brings us into the new basis. The new basis has quantum numbers $a = 1, 2, \dots, N$. Show that the new basis is orthonormal given that the old 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). Show also that the Slater determinants are orthogonal if we employ a single-particle basis which is orthogonal.