Exercises FYS4480, week 38, September 23-27, 2024

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.