

# Exercises FYS4480, week 40, September 30-October 4, 2024

## Exercise 1

Last week we considered a Slater determinant built up of single-particle orbitals  $\psi_\lambda$ , with  $\lambda = 1, 2, \dots, N$ . The unitary transformation

$$|a\rangle = \sum_{\lambda} C_{a\lambda} |\lambda\rangle,$$

brings us into the new basis. The new basis has quantum numbers  $a = 1, 2, \dots, N$ . We showed that the new basis is orthonormal given that the old basis is orthonormal and 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  $C$ . We showed then that the old and the new Slater determinants are equal up to a complex constant with absolute value unity. The resulting Slater determinants are orthogonal if we employ a single-particle basis which is orthogonal.

Define a Slater determinant  $|\Phi_0\rangle$  as an ansatz for the ground state using the single-particle basis functions  $|\mu\rangle$ . Assume that you have filled all states  $\mu$  up to the Fermi level and show that the expectation value for the ground state with a Hamiltonian that contains at most two-body interactions can be written as

$$\langle \Phi_0 | \hat{H} | \Phi_0 \rangle = \sum_{\mu=1}^N \langle \mu | \hat{h}_0 | \mu \rangle + \frac{1}{2} \sum_{\mu=1}^N \sum_{\nu=1}^N \langle \mu\nu | \hat{v} | \mu\nu \rangle_{AS}.$$

Explain what the different terms stand for and express the above equation in a diagrammatic form.

We define then a new Slater determinant  $|\Psi_0\rangle$  defined by the single-particle basis function  $|a\rangle$ , where the Fermi level is defined by filling all single-particle states  $a$  below the Fermi level. The new basis is also orthonormal.

Show that you can write the expectation value as

$$\langle \Psi_0 | \hat{H} | \Psi_0 \rangle = \sum_{i=1}^N \langle i | h | i \rangle + \frac{1}{2} \sum_{ij=1}^N \langle ij | \hat{v} | ij \rangle_{AS}.$$

Using the new single-particle basis  $|a\rangle$  (romans), show that you can rewrite the last equation in terms of the basis functions  $|\lambda\rangle$  (greek)

$$\langle \Psi_0 | \hat{H} | \Psi_0 \rangle = \sum_{i=1}^N \sum_{\alpha\beta} C_{i\alpha}^* C_{i\beta} \langle \alpha | h | \beta \rangle + \frac{1}{2} \sum_{ij=1}^N \sum_{\alpha\beta\gamma\delta} C_{i\alpha}^* C_{j\beta}^* C_{i\gamma} C_{j\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle_{AS}. \quad (1)$$