Exercises FYS4480, week 40, October 2-6, 2023

Exercise 1

Last week we considered a Slater determinant built up of single-particle orbitals ψ_λ, 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 fille all states μ 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 define 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 $|\lambda\rangle$ (greeks)

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