Exercises FYS4480, week 36, September 2-6, 2024

Exercise 1, Condon-Slater rules for expectation values

Consider three N-particle Slater determinants $|SD\rangle$, $|SD_i^j\rangle$ and $|SD_{ij}^{kl}\rangle$, where the notation means that Slater determinant $|SD_i^j\rangle$ differs from $|SD\rangle$ by one single-particle state, that is a single-particle state ψ_i is replaced by a single-particle state ψ_j. Similarly, the Slater determinant $|SD_{ij}^{kl}\rangle$ differs by two single-particle states from $|SD\rangle$.

We define thereafter a general onebody operator $\hat{F} = \sum_i^N \hat{f}(x_i)$ and a general twobody operator $\hat{G} = \sum_{i>j}^N \hat{g}(x_i, x_j)$ with g being invariant under the interchange of the coordinates of two particles. The single-particle states ψ_i are not necessarily eigenstates of $\hat{f}$.

a) Find the expectation values of

$$\langle SD|\hat{F}|SD\rangle,$$

and

$$\langle SD\hat{G}|SD\rangle.$$

b) Find thereafter t

$$\langle SD|\hat{F}|SD_i^j\rangle,$$

and

$$\langle SD\hat{G}|SD_i^j\rangle,$$

and finally

c) find

$$\langle SD|\hat{F}|SD_{ij}^{kl}\rangle,$$

and

$$\langle SD\hat{G}|SD_{ij}^{kl}\rangle.$$

What happens with the two-body operator if we have a transition probability of the type

$$\langle SD\hat{G}|SD_{ijk}^{lmn}\rangle,$$

where the Slater determinant to the right of the operator differs by more than two single-particle states?

Exercise 2, first second quantization encounter

a) Show that the density of particles with coordinates $\mathbf{x}$, is given by

$$n(\mathbf{x}) = N \int d\mathbf{x}_2 \dots d\mathbf{x}_N |\Psi_{AS}(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N)|^2$$

can be written in terms of the single-particle states ψ_k as

$$n(\mathbf{x}) = \sum_k |\psi_k(\mathbf{x})|^2.$$

b) Calculate the matrix elements (second quantization)

$$\langle\alpha_1\alpha_2|\,\hat{F}\,|\alpha_1\alpha_2\rangle$$

and

$$\langle\alpha_1\alpha_2|\,\hat{G}\,|\alpha_1\alpha_2\rangle$$

with

$$|\alpha_1\alpha_2\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\,|0\rangle\,,$$

$$\hat{F} = \sum_{\alpha\beta}\langle\alpha|\,f\,|\beta\rangle\,a^\dagger_\alpha a_\beta,$$

$$\langle\alpha|\,f\,|\beta\rangle = \int\psi^*_\alpha(x)f(x)\psi_\beta(x)dx,$$

$$\hat{G} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\,g\,|\gamma\delta\rangle\,a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma,$$

and

$$\langle\alpha\beta|\,g\,|\gamma\delta\rangle = \int\int\psi^*_\alpha(x_1)\psi^*_\beta(x_2)g(x_1,x_2)\psi_\gamma(x_1)\psi_\delta(x_2)dx_1dx_2$$

Compare these results with those from exercise 1c) from the exercise set of week 35.