b)

In this exercise we want to compute the matrix element

$$\langle a_1a_2a_3|G|b_1b_2b_3\rangle,$$

using second quantization notation and Wick's theorem. First, inserting for the two-body operator in second quantization and writing the states as vacuum states we have

$$\langle a_1a_2a_3|G|b_1b_2b_3\rangle = \frac{1}{2}\sum_{ijkl}\langle 0|\hat{a}_3\hat{a}_2\hat{a}_1\hat{i}^\dagger\hat{j}^\dagger\hat{k}\hat{l}\hat{b}_1^\dagger\hat{b}_2^\dagger\hat{b}_3^\dagger|0\rangle.$$

We now use Wick's theorem on the string of creation and annihilation operators. We know that only the terms where all the operators are contracted will contribute to the final result, and also that only contractions on the form $\alpha\beta^\dagger$ contribute.So Wick's theorem gives

$$\langle a_1a_2a_3|G|b_1b_2b_3\rangle = \frac{1}{2}\sum_{ijkl}\langle ij|\hat{g}|kl\rangle\langle 0|\Big(n\big[\hat{a}_3\hat{a}_2\hat{a}_1\hat{i}^\dagger\hat{j}^\dagger\hat{k}\hat{l}\hat{b}_1^\dagger\hat{b}_2^\dagger\hat{b}_3^\dagger\big]$$
$$+ n\big[\hat{a}_3\hat{a}_2\hat{a}_1\hat{i}^\dagger\hat{j}^\dagger\hat{k}\hat{l}\hat{b}_1^\dagger\hat{b}_2^\dagger\hat{b}_3^\dagger\big] + \dots\Big)$$

Let us look at what happens to such a normal product with contractions. Extracting each pair of operators we get

$$n\big[\hat{a}_3\hat{a}_2\hat{a}_1\hat{i}^\dagger\hat{j}^\dagger\hat{k}\hat{l}\hat{b}_1^\dagger\hat{b}_2^\dagger\hat{b}_3^\dagger\big] = \hat{a}_3\hat{i}^\dagger\hat{a}_2\hat{j}^\dagger\hat{a}_1\hat{b}_1^\dagger\hat{k}\hat{b}_2^\dagger\hat{l}\hat{b}_3^\dagger n\big[\big].$$

We now simplify this by realizing that the normal product of an empty operator string is just the identity operator, and also that the contraction $\hat{\alpha}\hat{\beta}^\dagger = \delta_{\alpha\beta}$. We get

$$n\big[\hat{a}_3\hat{a}_2\hat{a}_1\hat{i}^\dagger\hat{j}^\dagger\hat{k}\hat{l}\hat{b}_1^\dagger\hat{b}_2^\dagger\hat{b}_3^\dagger\big] = \delta_{a_3i}\delta_{a_2j}\delta_{a_1b_1}\delta_{kb_2}\delta_{lb_3}.$$

And when taking the sum over i, j, k and l, this term will contribute to the final matrix element as follows

$$\frac{1}{2}\sum_{ijkl}\langle ij|\hat{g}|kl\rangle\langle 0|n\big[\hat{a}_3\hat{a}_2\hat{a}_1\hat{i}^\dagger\hat{j}^\dagger\hat{l}\hat{k}\hat{b}_1^\dagger\hat{b}_2^\dagger\hat{b}_3^\dagger\big]|0\rangle = \frac{1}{2}\sum_{ijkl}\langle ij|\hat{g}|kl\rangle\delta_{a_3i}\delta_{a_2j}\delta_{a_1b_1}\delta_{kb_2}\delta_{lb_3}$$
$$= \frac{1}{2}\langle a_3a_2|\hat{g}|b_2b_3\rangle\delta_{a_1b_1}.$$

Now, this is just one of the terms. As there are 5 creation and 5 annihilation operators that must be contracted in the order $\hat{\alpha}\hat{\beta}^\dagger$—this gives a total of 36 normal products with contractions that contribute a term. We can write all these out by using SymPy, and the results are as follows.

$$\hat{C} =$$
$$+ \delta_{a_1b_1}\delta_{a_2i}\delta_{a_3j}\delta_{b_2k}\delta_{b_3l} - \delta_{a_1b_1}\delta_{a_2i}\delta_{a_3j}\delta_{b_2l}\delta_{b_3k} - \delta_{a_1b_1}\delta_{a_2j}\delta_{a_3i}\delta_{b_2k}\delta_{b_3l} + \delta_{a_1b_1}\delta_{a_2j}\delta_{a_3i}\delta_{b_2l}\delta_{b_3k}$$
$$- \delta_{a_1b_2}\delta_{a_2i}\delta_{a_3j}\delta_{b_1k}\delta_{b_3l} + \delta_{a_1b_2}\delta_{a_2i}\delta_{a_3j}\delta_{b_1l}\delta_{b_3k} + \delta_{a_1b_2}\delta_{a_2j}\delta_{a_3i}\delta_{b_1k}\delta_{b_3l} - \delta_{a_1b_2}\delta_{a_2j}\delta_{a_3i}\delta_{b_1l}\delta_{b_3k}$$
$$+ \delta_{a_1b_3}\delta_{a_2i}\delta_{a_3j}\delta_{b_1k}\delta_{b_2l} - \delta_{a_1b_3}\delta_{a_2i}\delta_{a_3j}\delta_{b_1l}\delta_{b_2k} - \delta_{a_1b_3}\delta_{a_2j}\delta_{a_3i}\delta_{b_1k}\delta_{b_2l} + \delta_{a_1b_3}\delta_{a_2j}\delta_{a_3i}\delta_{b_1l}\delta_{b_2k}$$
$$- \delta_{a_1i}\delta_{a_2b_1}\delta_{a_3j}\delta_{b_2k}\delta_{b_3l} + \delta_{a_1i}\delta_{a_2b_1}\delta_{a_3j}\delta_{b_2l}\delta_{b_3k} + \delta_{a_1i}\delta_{a_2b_2}\delta_{a_3j}\delta_{b_1k}\delta_{b_3l} - \delta_{a_1i}\delta_{a_2b_2}\delta_{a_3j}\delta_{b_1l}\delta_{b_3k}$$
$$- \delta_{a_1i}\delta_{a_2b_3}\delta_{a_3j}\delta_{b_1k}\delta_{b_2l} + \delta_{a_1i}\delta_{a_2b_3}\delta_{a_3j}\delta_{b_1l}\delta_{b_2k} + \delta_{a_1i}\delta_{a_2j}\delta_{a_3b_1}\delta_{b_2k}\delta_{b_3l} - \delta_{a_1i}\delta_{a_2j}\delta_{a_3b_1}\delta_{b_2l}\delta_{b_3k}$$
$$- \delta_{a_1i}\delta_{a_2j}\delta_{a_3b_2}\delta_{b_1k}\delta_{b_3l} + \delta_{a_1i}\delta_{a_2j}\delta_{a_3b_2}\delta_{b_1l}\delta_{b_3k} + \delta_{a_1i}\delta_{a_2j}\delta_{a_3b_3}\delta_{b_1k}\delta_{b_2l} - \delta_{a_1i}\delta_{a_2j}\delta_{a_3b_3}\delta_{b_1l}\delta_{b_2k}$$
$$+ \delta_{a_1j}\delta_{a_2b_1}\delta_{a_3i}\delta_{b_2k}\delta_{b_3l} - \delta_{a_1j}\delta_{a_2b_1}\delta_{a_3i}\delta_{b_2l}\delta_{b_3k} - \delta_{a_1j}\delta_{a_2b_2}\delta_{a_3i}\delta_{b_1k}\delta_{b_3l} + \delta_{a_1j}\delta_{a_2b_2}\delta_{a_3i}\delta_{b_1l}\delta_{b_3k}$$
$$+ \delta_{a_1j}\delta_{a_2b_3}\delta_{a_3i}\delta_{b_1k}\delta_{b_2l} - \delta_{a_1j}\delta_{a_2b_3}\delta_{a_3i}\delta_{b_1l}\delta_{b_2k} - \delta_{a_1j}\delta_{a_2i}\delta_{a_3b_1}\delta_{b_2k}\delta_{b_3l} + \delta_{a_1j}\delta_{a_2i}\delta_{a_3b_1}\delta_{b_2l}\delta_{b_3k}$$
$$+ \delta_{a_1j}\delta_{a_2i}\delta_{a_3b_2}\delta_{b_1k}\delta_{b_3l} - \delta_{a_1j}\delta_{a_2i}\delta_{a_3b_2}\delta_{b_1l}\delta_{b_3k} - \delta_{a_1j}\delta_{a_2i}\delta_{a_3b_3}\delta_{b_1k}\delta_{b_2l} + \delta_{a_1j}\delta_{a_2i}\delta_{a_3b_3}\delta_{b_1l}\delta_{b_2k}$$

We can treat each of these terms as we have above. When taking the sum over i, j, k and l, we get the following contributions to the final matrix element

$$\frac{1}{2}\sum_{ijkl}\langle ij|\hat{g}|kl\rangle\langle 0|\hat{C}|0\rangle = \frac{1}{2}\big($$

$$\begin{aligned}
&+ \langle a_2a_3|\hat{g}|b_2b_3\rangle\delta_{a_1b_1} - \langle a_2a_3|\hat{g}|b_3b_2\rangle\delta_{a_1b_1} - \langle a_3a_2|\hat{g}|b_2b_3\rangle\delta_{a_1b_1} + \langle a_3a_2|\hat{g}|b_3b_2\rangle\delta_{a_1b_1}\\
&- \langle a_2a_3|\hat{g}|b_1b_3\rangle\delta_{a_1b_2} + \langle a_2a_3|\hat{g}|b_3b_1\rangle\delta_{a_1b_2} + \langle a_3a_2|\hat{g}|b_1b_3\rangle\delta_{a_1b_2} - \langle a_3a_2|\hat{g}|b_3b_1\rangle\delta_{a_1b_2}\\
&+ \langle a_2a_3|\hat{g}|b_1b_2\rangle\delta_{a_1b_3} - \langle a_2a_3|\hat{g}|b_2b_1\rangle\delta_{a_1b_3} - \langle a_3a_2|\hat{g}|b_1b_2\rangle\delta_{a_1b_3} + \langle a_3a_2|\hat{g}|b_2b_1\rangle\delta_{a_1b_3}\\
&- \langle a_1a_3|\hat{g}|b_2b_3\rangle\delta_{a_2b_1} + \langle a_1a_3|\hat{g}|b_3b_2\rangle\delta_{a_2b_1} + \langle a_3a_1|\hat{g}|b_2b_3\rangle\delta_{a_2b_1} - \langle a_3a_1|\hat{g}|b_3b_2\rangle\delta_{a_2b_1}\\
&+ \langle a_1a_3|\hat{g}|b_1b_3\rangle\delta_{a_2b_2} - \langle a_1a_3|\hat{g}|b_3b_1\rangle\delta_{a_2b_2} - \langle a_3a_1|\hat{g}|b_1b_3\rangle\delta_{a_2b_2} + \langle a_3a_1|\hat{g}|b_3b_1\rangle\delta_{a_2b_2}\\
&- \langle a_1a_3|\hat{g}|b_1b_2\rangle\delta_{a_2b_3} + \langle a_1a_3|\hat{g}|b_2b_1\rangle\delta_{a_2b_3} + \langle a_3a_1|\hat{g}|b_1b_2\rangle\delta_{a_2b_3} - \langle a_3a_1|\hat{g}|b_2b_1\rangle\delta_{a_2b_3}\\
&+ \langle a_1a_2|\hat{g}|b_2b_3\rangle\delta_{a_3b_1} - \langle a_1a_2|\hat{g}|b_3b_2\rangle\delta_{a_3b_1} - \langle a_2a_1|\hat{g}|b_2b_3\rangle\delta_{a_3b_1} + \langle a_2a_1|\hat{g}|b_3b_2\rangle\delta_{a_3b_1}\\
&+ \langle a_2a_1|\hat{g}|b_1b_3\rangle\delta_{a_3b_2} - \langle a_2a_1|\hat{g}|b_3b_1\rangle\delta_{a_3b_2} - \langle a_1a_2|\hat{g}|b_1b_3\rangle\delta_{a_3b_2} + \langle a_1a_2|\hat{g}|b_3b_1\rangle\delta_{a_3b_2}\\
&+ \langle a_1a_2|\hat{g}|b_1b_2\rangle\delta_{a_3b_3} - \langle a_1a_2|\hat{g}|b_2b_1\rangle\delta_{a_3b_3} - \langle a_2a_1|\hat{g}|b_1b_2\rangle\delta_{a_3b_3} + \langle a_2a_1|\hat{g}|b_2b_1\rangle\delta_{a_3b_3}\big).
\end{aligned}$$

We note that every line consists of four terms with the same Kroneckerqdelta indices, we can collect these terms in each case. We can also use the the fact that generally

$$\langle\alpha\beta|\hat{q}|\gamma\delta\rangle = \langle\beta\alpha|\hat{q}|\delta\gamma\rangle,$$

to combine two and two of the terms. Let us look at the first line as an example

$$\frac{1}{2}\big(\langle a_2a_3|\hat{g}|b_2b_3\rangle - \langle a_2a_3|\hat{g}|b_3b_2\rangle - \langle a_3a_2|\hat{g}|b_2b_3\rangle + \langle a_3a_2|\hat{g}|b_3b_2\rangle\big)\delta_{a_1b_1}.$$

Which can be simplified to

$$\big(\langle a_2a_3|\hat{g}|b_2b_3\rangle - \langle a_2a_3|\hat{g}|b_3b_2\rangle\big)\delta_{a_1b_1}.$$

Which can be written even more compactily as

$$\langle a_2a_3|\hat{g}|b_2b_3\rangle_{\mathrm{AS}}\delta_{a_1b_1}.$$

By using the same simplification for each line, we get the final result

$$\begin{aligned}
\langle a_1a_2a_3|G|b_1b_2b_3\rangle = &\langle a_2a_3|\hat{g}|b_2b_3\rangle_{\mathrm{AS}}\delta_{a_1b_1}\\
&+ \langle a_2a_3|\hat{g}|b_3b_1\rangle_{\mathrm{AS}}\delta_{a_1b_2}\\
&+ \langle a_2a_3|\hat{g}|b_1b_2\rangle_{\mathrm{AS}}\delta_{a_1b_3}\\
&+ \langle a_1a_3|\hat{g}|b_3b_2\rangle_{\mathrm{AS}}\delta_{a_2b_1}\\
&+ \langle a_1a_3|\hat{g}|b_1b_3\rangle_{\mathrm{AS}}\delta_{a_2b_2}\\
&+ \langle a_1a_3|\hat{g}|b_2b_1\rangle_{\mathrm{AS}}\delta_{a_2b_3}\\
&+ \langle a_1a_2|\hat{g}|b_2b_3\rangle_{\mathrm{AS}}\delta_{a_3b_1}\\
&+ \langle a_1a_2|\hat{g}|b_3b_1\rangle_{\mathrm{AS}}\delta_{a_3b_2}\\
&+ \langle a_1a_2|\hat{g}|b_1b_2\rangle_{\mathrm{AS}}\delta_{a_3b_3}
\end{aligned}$$

We can test our result by looking at our results from last week, where we looked at the matrix elements for general n-particle Slater determinants with zero, one, two and three-noncoincidences, which were as follows

$$\begin{aligned}
\langle SD|\hat{G}|SD\rangle &= \frac{1}{2}\sum_{\alpha,\beta}\langle\alpha\beta|\hat{g}|\alpha\beta\rangle_{\mathrm{AS}},\\
\langle SD|\hat{G}|SD_i^j\rangle &= \sum_{\alpha}\langle\alpha i|\hat{g}|\alpha j\rangle_{\mathrm{AS}},\\
\langle SD|\hat{G}|SD_{ij}^{kl}\rangle &= \langle ij|\hat{g}|kl\rangle_{\mathrm{AS}},\\
\langle SD|\hat{G}|SD_{ijl}^{lmn}\rangle &= 0.
\end{aligned}$$

Zero noncoincidences

In our case, if there are zero noncoincidences, it means that $\{a_1, a_2, a_3\} = \{b_1, b_2, b_3\}$. Note that these sets are not ordered, meaning the a's can be permuted in relation to the b's. The simplest case to look at is $a_1 = b_1$, $a_2 = b_2$ and $a_3 = b_3$. Our results from last week then gives

$$\begin{aligned}\langle SD|\hat{G}|SD\rangle &= \frac{1}{2}\sum_{\alpha,\beta}\langle\alpha\beta|\hat{g}|\alpha\beta\rangle_{\text{AS}} \\ &= \frac{1}{2}\big[\langle 11|\hat{g}|11\rangle_{\text{AS}} + \langle 12|\hat{g}|12\rangle_{\text{AS}} + \langle 13|\hat{g}|13\rangle_{\text{AS}} \\ &\quad + \langle 21|\hat{g}|21\rangle_{\text{AS}} + \langle 22|\hat{g}|22\rangle_{\text{AS}} + \langle 23|\hat{g}|23\rangle_{\text{AS}} \\ &\quad + \langle 31|\hat{g}|31\rangle_{\text{AS}} + \langle 32|\hat{g}|32\rangle_{\text{AS}} + \langle 33|\hat{g}|33\rangle_{\text{AS}}.\end{aligned}$$

Where we have introduced the shorthand $\langle ij|\hat{g}|ij\rangle \equiv \langle a_i a_j|\hat{g}|b_i b_j\rangle$. We now use the properties

$$\langle ii|\hat{g}|ii\rangle = 0 \quad \text{and} \quad \langle ij|\hat{q}|ij\rangle = \langle ji|\hat{q}|ji\rangle,$$

which gives

$$\langle a_1 a_2 a_3|\hat{G}|a_1 a_2 a_3\rangle = \langle 12|\hat{g}|12\rangle_{\text{AS}} + \langle 13|\hat{g}|13\rangle_{\text{AS}} + \langle 23|\hat{g}|23\rangle_{\text{AS}}.$$

Which fits perfectly with out result this week. Note also that if we had permuted any of the b's relative to the a's, we would still have three terms in the result.

One noncoincidence

We now let $a_1 = b_1$ and $a_2 = b_2$, but $a_3 \neq b_3$. Our result from this week would then be

$$\langle a_1 a_2 a_3|\hat{G}|a_1 a_2 b_3\rangle = \langle 13|\hat{g}|13\rangle_{\text{AS}} + \langle 23|\hat{g}|23\rangle_{\text{AS}}.$$

From the previous week, this corresponds to

$$\langle SD|\hat{G}|SD_{a_3}^{b_3}\rangle = \sum_{\alpha}\langle\alpha a_3|\hat{g}|\alpha b_3\rangle_{\text{AS}} = \langle 13|\hat{g}|13\rangle_{\text{AS}} + \langle 23|\hat{g}|23\rangle_{\text{AS}}.$$

Two noncoincidences

Letting $a_1 = b_1$, but $a_2 \neq b_2$ and $a_3 \neq b_3$, we see that only the first term in our result survives, and we have

$$\langle a_1 a_2 a_3|\hat{G}|a_1 b_2 b_3\rangle = \langle 23|\hat{g}|23\rangle_{\text{AS}}.$$

From last weeks result we have

$$\langle SD|\hat{G}|SD_{a_2 a_3}^{b_2 b_3}\rangle = \langle 23|\hat{g}|23\rangle_{\text{AS}},$$

and we see the two results are equal, as expected.

Three noncoincidences

If none of the single-particle states are equal, we see that all of the Kronecker-deltas vanish, and the result is zero, just as we expected from last week.