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1 Deriving complicated spin integration

We are trying to get from

$$W_{p,q,i,a} = \sum_{\underline{p,q,i,a}} (\underline{pq}|\underline{ia}) \tag{1}$$

to

$$W_{p,q,i,a} = \sqrt{2} \sum_{p,q,i,a} (pq|ia) \tag{2}$$

This deprecation will require work in second quantization using weeks thm: We start with the two electron operator in second quantization:

$$\hat{V} = \frac{1}{4} \sum_{pqrs} V_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r \tag{3}$$

We are interested in how this acts on the singlet CSF:

$$|\Psi_S\rangle = \frac{1}{\sqrt{2}} (a_a^{\alpha\dagger} a_i^\alpha + a_a^{\beta\dagger} a_i^\beta) \tag{4}$$

We act the operator on the singled state and use Wick's theorem to simplify:

$$\hat{V} |\Psi_S\rangle = \frac{1}{4} \sum_{pqrs} V_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r \frac{1}{\sqrt{2}} (a_a^{\alpha\dagger} a_i^\alpha + a_a^{\beta\dagger} a_i^\beta) \tag{5}$$

$$\hat{V} |\Psi_S\rangle = \frac{1}{4} \sum_{pqrs} V_{pqrs} \frac{1}{\sqrt{2}} \left(\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r a_a^{\alpha\dagger} a_i^\alpha + \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r a_a^{\beta\dagger} a_i^\beta \right) \tag{6}$$