Documentation for Developers

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Tensor Conventions

Both the gradient and trial vectors are considered in terms of dictionaries of "blocks" following spin-integration, with redundancy coming only from the antisymmetry condition. Each four-tensor and two-tensor "block" B will have

$$|\psi_{ij}^{ab}\rangle \rightarrow B_{ijab}$$

and

$$|\psi_{i}^{a}\rangle \rightarrow B_{ia}$$

respectively. The overall structure of a vector will look like:

$$\begin{pmatrix} S_\alpha \\ S_\beta \\ D_{\alpha\alpha} \\ D_{\alpha\beta} \\ D_{\beta\alpha} \\ D_{\beta\beta} \end{pmatrix}$$

where each S is a two-tensor of single excitations, and each D is a four-tensor of double excitations. To avoid ambiguity, double excitations will be mapped as:

$$|\psi_{\alpha\beta}^{\alpha\beta}\rangle \rightarrow D_{\alpha\beta}$$

The Hessian is composed of 36 blocks:

$$\hat{\eta} = \begin{pmatrix} S_\alpha/S_\alpha & S_\alpha/S_\beta & S_\alpha/D_{\alpha\alpha} & S_\alpha/D_{\alpha\beta} & S_\alpha/D_{\beta\alpha} & S_\alpha/D_{\beta\beta} \\ S_\beta/S_\alpha & S_\beta/S_\beta & S_\beta/D_{\alpha\alpha} & S_\beta/D_{\alpha\beta} & S_\beta/D_{\beta\alpha} & S_\beta/D_{\beta\beta} \\ D_{\alpha\alpha}/S_\alpha & D_{\alpha\alpha}/S_\beta & D_{\alpha\alpha}/D_{\alpha\alpha} & D_{\alpha\alpha}/D_{\alpha\beta} & D_{\alpha\alpha}/D_{\beta\alpha} & D_{\alpha\alpha}/D_{\beta\beta} \\ D_{\alpha\beta}/S_\alpha & D_{\alpha\beta}/S_\beta & D_{\alpha\beta}/D_{\alpha\alpha} & D_{\alpha\beta}/D_{\alpha\beta} & D_{\alpha\beta}/D_{\beta\alpha} & D_{\alpha\beta}/D_{\beta\beta} \\ D_{\beta\alpha}/S_\alpha & D_{\beta\alpha}/S_\beta & D_{\beta\alpha}/D_{\alpha\alpha} & D_{\beta\alpha}/D_{\alpha\beta} & D_{\beta\alpha}/D_{\beta\alpha} & D_{\beta\alpha}/D_{\beta\beta} \\ D_{\beta\beta}/S_\alpha & D_{\beta\beta}/S_\beta & D_{\beta\beta}/D_{\alpha\alpha} & D_{\beta\beta}/D_{\alpha\beta} & D_{\beta\beta}/D_{\beta\alpha} & D_{\beta\beta}/D_{\beta\beta} \end{pmatrix}$$

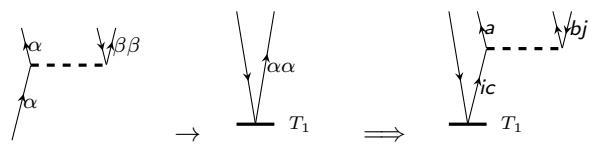
As an example, consider the S_α block of the action, $\vec{a}$, of $\hat{\eta}$ on a trial vector $\hat{\theta}$.

$$S_\alpha^{\vec{a}} = \begin{pmatrix} S_\alpha/S_\alpha & S_\alpha/S_\beta & S_\alpha/D_{\alpha\alpha} & S_\alpha/D_{\alpha\beta} & S_\alpha/D_{\beta\alpha} & S_\alpha/D_{\beta\beta} \end{pmatrix}^{\hat{\eta}} \begin{pmatrix} S_\alpha \\ S_\beta \\ D_{\alpha\alpha} \\ D_{\alpha\beta} \\ D_{\beta\alpha} \\ D_{\beta\beta} \end{pmatrix}^{\vec{\theta}}$$

where the dot product operator is spin-integrated tensor contraction instead of multiplication. This arithmetic is easily generalized to vector multiplications. For the sake of explicitness, we consider the

$$D_{\alpha\beta}/S_{\alpha}^{\hat{\eta}} \rightarrow S_{\alpha}^{\vec{\theta}} \implies D_{\alpha\beta}^{\vec{a}}$$

contraction, specifically the following contraction:



Note that we place α q-particles on the left and β q-particles on the right to be consistent with the fact that we want to recover part of the $D_{\alpha\beta}$ action from this contraction. This is mostly pedagogical, as it makes it easier to keep track of things like permutations. In general, this contraction looks like would contribute

$$\vec{a}_{ijcb} = \sum_{c} \mathcal{P}_{ij} \langle ab||cj\rangle \vec{\theta}_{ic}$$

However, we wish to spin-integrate this. First, we note that the exchange contribution will be 0 because a and j are of opposite spins. (As are b and c). Additionally, we know that permuting i and j will lead to the requirement that a β hole line is entering T_1. Therefore, this term reduces to:

$$\vec{a}_{ijcb} = \sum_{c} \langle ab|cj\rangle \vec{\theta}_{ic}$$

Note that for consistency, our vector elements are read from diagrams as in-in-out-out.