PAO LNV for arbitrary A and B matrices

The LNV energy functional is:

$$\Omega = 3\,\mathrm{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{H}] - 2\,\mathrm{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{S}\tilde{P}\tilde{H}]$$

The tilded variables are in the smaller PAO-basis. The transformations between the larger primary basis and the PAO-basis are:

$$\tilde{P} = A^T P A \qquad \tilde{H} = B^T H B \qquad \tilde{S} = B^T S B$$

Notice that: $A^T B = B^T A = \tilde{I}$, where $\tilde{I}$ is the identity matrix in the smaller PAO basis.

The relationship between A and B is defined via the Moore-Penrose pseudo-inverse:

$$B = S^{-1} A (A^T S^{-1} A)^{-1}$$

1. Derivative

$$
\begin{aligned}
\frac{d\Omega}{dA_{ij}} &= \sum_{ab} \frac{\partial \Omega}{\partial \tilde{P}_{ab}} \frac{\partial \tilde{P}_{ab}}{\partial A_{ij}} + \sum_{ab} \frac{\partial \Omega}{\partial \tilde{H}_{ab}} \frac{\partial \tilde{H}_{ab}}{\partial A_{ij}} + \sum_{ab} \frac{\partial \Omega}{\partial \tilde{S}_{ab}} \frac{\partial \tilde{S}_{ab}}{\partial A_{ij}} \\
&= \sum_{ab} M^1_{ab} \frac{\partial \tilde{P}_{ab}}{\partial A_{ij}} + \sum_{ab} M^2_{ab} \frac{\partial \tilde{H}_{ab}}{\partial A_{ij}} + \sum_{ab} M^3_{ab} \frac{\partial \tilde{S}_{ab}}{\partial A_{ij}} \\
&= T^1_{ij} + T^2_{ij} + T^3_{ij}
\end{aligned}
$$

$$
\begin{aligned}
T^1_{ij} &= \sum_{ab} M^1_{ab} \frac{\partial \tilde{P}_{ab}}{\partial A_{ij}} \\
&= \sum_{ablk} M^1_{ab} \frac{\partial}{\partial A_{ij}} A_{la} P_{lk} A_{kb} \\
&= \sum_{ablk} M^1_{ab} \left[\delta_{li} \delta_{aj} P_{lk} A_{kb} + A_{la} P_{lk} \delta_{ki} \delta_{bj} \right] \\
&= \left[PAM^{1T} \right]_{ij} + \left[P^T A M^1 \right]_{ij} \\
&= 2 \left[PAM^1 \right]_{ij}
\end{aligned}
$$

$$
T^2_{ij} = \sum_{ab} R^2_{ab} \frac{\partial B_{ab}}{\partial A_{ij}}
$$

$$
T^3_{ij} = \sum_{ab} R^3_{ab} \frac{\partial B_{ab}}{\partial A_{ij}}
$$

$$
\begin{aligned}
R^2_{ij} &= \sum_{ab} M^2_{ab} \frac{\partial \tilde{H}_{ab}}{\partial B_{ij}} \\
&= \sum_{ablk} M^2_{ab} \frac{\partial}{\partial B_{ij}} B_{la} H_{lk} B_{kb} \\
&= \sum_{ablk} M^2_{ab} \left[\delta_{li}\delta_{aj} H_{lk} B_{kb} + \delta_{ki}\delta_{bj} B_{la} H_{lk}\right] \\
&= \left[HBM^{2T}\right]_{ij} + \left[H^T BM^2\right]_{ij} \\
&= 2\left[HBM^2\right]_{ij}
\end{aligned}
$$

Educated guess:

$$
\begin{aligned}
R^3_{ij} &= \sum_{ab} M^3_{ab} \frac{\partial \tilde{S}_{ab}}{\partial B_{ij}} \\
&= 2\left[SBM^3\right]_{ij}
\end{aligned}
$$

$$
\begin{aligned}
M^1_{ab} &= \frac{\partial \Omega}{\partial \tilde{P}_{ab}} \\
&= \frac{\partial}{\partial \tilde{P}_{ab}} \Big(3\,\mathrm{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{H}] - 2\,\mathrm{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{S}\tilde{P}\tilde{H}] \Big) \\
&= 3\tilde{H}\tilde{P}\tilde{S} + 3\tilde{S}\tilde{P}\tilde{H} - 2\tilde{H}\tilde{P}\tilde{S}\tilde{P}\tilde{S} - 2\tilde{S}\tilde{P}\tilde{H}\tilde{P}\tilde{S} - 2\tilde{S}\tilde{P}\tilde{S}\tilde{P}\tilde{H}
\end{aligned}
$$

$$
\begin{aligned}
M^2_{ab} &= \frac{\partial \Omega}{\partial \tilde{H}_{ab}} \\
&= \frac{\partial}{\partial \tilde{H}_{ab}} \Big(3\,\mathrm{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{H}] - 2\,\mathrm{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{S}\tilde{P}\tilde{H}] \Big) \\
&= 3\tilde{P}\tilde{S}\tilde{P} - 2\tilde{P}\tilde{S}\tilde{P}\tilde{S}\tilde{P}
\end{aligned}
$$

$$
\begin{aligned}
M^3_{ab} &= \frac{\partial \Omega}{\partial \tilde{S}_{ab}} \\
&= \frac{\partial}{\partial \tilde{S}_{ab}} \Big(3\,\mathrm{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{H}] - 2\,\mathrm{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{S}\tilde{P}\tilde{H}] \Big) \\
&= 3\tilde{P}\tilde{H}\tilde{P} - 2\tilde{P}\tilde{H}\tilde{P}\tilde{S}\tilde{P} - 2\tilde{P}\tilde{S}\tilde{P}\tilde{H}\tilde{P}
\end{aligned}
$$