1 Z-Vector Equation (Matrix Parameterization)

Imposing the stationary condition on the Lagrangian w.r.t. the orbital rotation parameter: (Usually take the linear combination of f_{ai} and f^*_{ia} to make the Lagrangian real, and remember that the fock matrix is Hermitian.)
In Matrix Parameterization, C_{ON} is required!

$$\begin{aligned}
\mathcal{L}_{\mathrm{MP2}} =& E_{\mathrm{HF}} + E_{\mathrm{H}} + \sum_{ai} z_{ai} f_{ai} \\
=& \sum_{pq} h_{pq}\gamma_{pq} + \sum_{pqrs} \Gamma^{pq}_{rs} \langle pq||rs\rangle + \sum_{ai} z_{ai} f_{ai} \\
=& \sum_{pq} h_{pq}\gamma^{\mathrm{HF}}_{pq} + \sum_{pqrs} (\Gamma^{pq}_{rs})^{\mathrm{HF}} \langle pq||rs\rangle \\
&+ \sum_{pq} h_{pq}\gamma^{\mathrm{H}}_{pq} + \sum_{pqrs} (\Gamma^{pq}_{rs})^{\mathrm{H}} \langle pq||rs\rangle + \sum_{ai} z_{ai} f_{ai}
\end{aligned} \tag{1}$$

$$\frac{\partial \mathcal{L}_{\mathrm{MP2}}}{\partial \mathbf{U}} = \frac{\partial E_{\mathrm{HF}}}{\partial \mathbf{U}} + \frac{\partial E_{\mathrm{H}}}{\partial \mathbf{U}} + \sum_{ai} z_{ai} \frac{\partial f_{ai}}{\partial \mathbf{U}} = 0 \tag{2}$$

The Hylleraas part (assuming real):

$$E_{\mathrm{H}} = \sum_{ij} h_{ij}\gamma_{ij} + \sum_{ab} h_{ab}\gamma_{ab} + \sum_{ijab} \langle ab||ij\rangle \Gamma^{ab}_{ij} + \sum_{ijkl} \langle ij||kl\rangle \Gamma^{ij}_{kl} + \sum_{ijab} \langle ai||bj\rangle \Gamma^{ai}_{bj} \tag{3}$$

Which blocks of $\mathbf{U}$ should be considered?
In general, all of them! But some will come out to be redundant and the ones contribute are the virtual-occupied blocks.
Also, need to take linear combination of $\frac{\partial}{\partial U_{pq}}$ and $\frac{\partial}{\partial U^*_{qp}}$ to get rid of the Lagrange multilpier in C_{ON} condition.
Could treat $\mathbf{U}$ and $\mathbf{U}^*$ as independent variables, i.e.:

$$\frac{\partial U_{pq}}{\partial U^*_{rs}} = 0 \tag{4}$$

Or just treat real and imaginary parts separately.

$$\begin{aligned}
\frac{\partial h_{ij}}{\partial U_{pq}} =& \frac{\partial}{\partial U_{pq}} \sum_{\mu\nu} C^*_{\mu i} h_{\mu\nu} C_{\nu j} \\
=& \frac{\partial}{\partial U_{pq}} \sum_{\mu\nu rs} C^*_{\mu r}(0) U^*_{ri} h_{\mu\nu} C_{\nu s}(0) U_{sj} \\
=& \sum_{\mu\nu r} C^*_{\mu r}(0) \frac{\partial U^*_{ri}}{\partial U_{pq}} h_{\mu\nu} C_{\nu j} + \sum_{\mu\nu r} C^*_{\mu i} h_{\mu\nu} C_{\nu r}(0) \frac{\partial U_{rj}}{\partial U_{pq}} \\
=& 0 + \sum_{\mu\nu r} C^*_{\mu i} h_{\mu\nu} C_{\nu r}(0) \delta_{pr}\delta_{qj} \\
=& \sum_{\mu\nu} C^*_{\mu i} h_{\mu\nu} C_{\nu p}(0) \delta_{qj}
\end{aligned} \tag{5}$$

Similarly:

$$\frac{\partial h_{ab}}{\partial U_{pq}} = \sum_{\mu\nu r} C^*_{\mu r}(0) (\frac{\partial U_{ra}}{\partial U_{pq}})^* h_{\mu\nu} C_{\nu b} + \sum_{\mu\nu r} C^*_{\mu a} h_{\mu\nu} C_{\nu r}(0) \frac{\partial U_{rb}}{\partial U_{pq}} \tag{6}$$

$$
\begin{aligned}
\frac{\partial\langle ab||ij\rangle}{\partial U_{pq}} =& \frac{\partial}{\partial U_{pq}}\sum_{\mu\nu\sigma\tau} C^*_{\mu a}C^*_{\nu b}\langle\mu\nu||\sigma\tau\rangle C_{\sigma i}C_{\tau j} \\
=& \sum_{\mu\nu\sigma\tau r} C^*_{\mu r}(0)(\frac{\partial U_{ra}}{\partial U_{pq}})^* C^*_{\nu b}\langle\mu\nu||\sigma\tau\rangle C_{\sigma i}C_{\tau j} \\
&+ \sum_{\mu\nu\sigma\tau r} C^*_{\mu a}C^*_{\nu r}(0)(\frac{\partial U_{rb}}{\partial U_{pq}})^*\langle\mu\nu||\sigma\tau\rangle C_{\sigma i}C_{\tau j} \\
&+ \sum_{\mu\nu\sigma\tau r} C^*_{\mu a}C^*_{\nu b}\langle\mu\nu||\sigma\tau\rangle C_{\sigma r}(0)\frac{\partial U_{ri}}{\partial U_{pq}}C_{\tau j} \\
&+ \sum_{\mu\nu\sigma\tau r} C^*_{\mu a}C^*_{\nu b}\langle\mu\nu||\sigma\tau\rangle C_{\sigma i}C_{\tau r}(0)\frac{\partial U_{rj}}{\partial U_{pq}}
\end{aligned} \tag{7}
$$

Other blocks of the 2e-integrals are similar.
note:

$$
\frac{\mathrm{d}U_{pq}}{\mathrm{d}U_{rs}} = \delta_{pr}\delta_{qs} \tag{8}
$$

Now the Brillouin part:

$$
\frac{\partial f_{ai}}{\partial U_{pq}} = \frac{\partial}{\partial U_{pq}}\left(h_{ai} + \sum_j \langle aj||ij\rangle\right) \tag{9}
$$

The constituent parts have been worked out from above.