Consider the AO basis set ϕ_μ, with overlap matrix $S_{\mu\nu} = \langle\phi_\mu|\phi_\nu\rangle$

The relationship between the density and the density matrix is basically:

$$\rho(r) = \sum_{\mu\nu} P_{\mu\nu}\phi_\mu^*\phi_\nu$$

Consider the Lowdin orthogonalization, define the new orthogonalized basis:

$$\begin{aligned}\bar{\phi}_\mu &= X_{\mu\nu}\phi_\nu \\ X_{\mu\nu} &= S_{\mu\nu}^{-1/2} \\ \phi_\mu &= X_{\mu\nu}^{-1}\bar{\phi}_\nu\end{aligned}$$

Obviously:

$$\left\langle\bar{\phi}_\mu\middle|\bar{\phi}_\nu\right\rangle = \sum_{\alpha\beta} X_{\mu\alpha}X_{\nu\beta}\langle\phi_\alpha|\phi_\beta\rangle = XSX^T = I$$

Then we intend to write the density matrix in the orthogonalized basis:

$$\begin{aligned}\rho(r) &= \sum_{\alpha\beta} P_{\alpha\beta}\phi_\alpha^*\phi_\beta \\ &= \sum_{\mu\nu}\sum_{\alpha\beta} P_{\alpha\beta}X_{\alpha\mu}^{-1}\bar{\phi}_\mu^*X_{\beta\nu}^{-1}\bar{\phi}_\nu \\ &= \sum_{\mu\nu}\bar{P}_{\mu\nu}\bar{\phi}_\mu^*\bar{\phi}_\nu\end{aligned}$$

With (considering X must be symmetric):

$$\bar{P} = X^{-1}PX^{-1}$$

Then what you need to do is the following:

1. Find the total density matrix in the overlap subspace:

$$P = P_A + P_B$$

2. Find the P in orthogonalized basis:

$$\bar{P} = X^{-1}PX^{-1}$$

3. Diagonalize $\bar{P}$, and decompose it into cluster and environment parts according to the eigenvalues:

$$\begin{aligned}\bar{P} &= U^TDU \\ &= U^T(D_A + D_B)U \\ &= U^TD_AU + U^TD_BU \\ &= \bar{P}_A' + \bar{P}_B'\end{aligned}$$

Here, D_A keeps all the diagonal elements that are 0.5, while D_B keeps all the diagonal elements that are 1.

4. Rotate back to normal AO basis:

$$
\begin{aligned}
P'_A &= X\bar{P}'_A X \\
P'_B &= X\bar{P}'_A X
\end{aligned}
$$

5. Do OEP to reproduce P'_A, maximize the following functional to find the embedding potential V_{emb}:

$$
W[V] = E_A[V] + \sum_{\mu\nu} V_{\mu\nu}\big(P[V] - P'_A\big)_{\mu\nu}
$$

   Here $P[V]$ is the density matrix coming from the embedded DFT calculation.

6. Use the P'_B to construct the projection potential:

$$
V_P = \mu S P'_B S
$$

7. Finally, the full embedding potential is:

$$
\begin{aligned}
V &= V_{emb} + V_P \\
&= V_{emb} + \mu S P'_B S
\end{aligned}
$$