Supplementary Material for: Negativity of the target density in practical Frozen-Density Embedding Theory based calculations

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I. APPENDIX: BOUNDARIES OF $P[\rho_A^o + \rho_B - \rho_{AB}^o]$

The parameter P is bound by:

$$M[\rho_B - \rho_{AB}^o] \leq P[\rho_A^o + \rho_B - \rho_{AB}^o] \leq N_{AB}. \tag{1}$$

Due to the fact that:

$$\int \rho_A^o + \rho_B = \int \rho_{AB}^o = N_{AB}, \tag{2}$$

where N_{AB} is the number of electrons of the supersystem, the integrated difference of these two densities is zero:

$$\begin{aligned}
&\int \rho_A^o + \rho_B - \rho_{AB}^o = 0 \\
&\int\limits_{\rho_{AB}^o < \rho_A^o + \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o + \int\limits_{\rho_{AB}^o > \rho_A^o + \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o = 0 \\
&\int\limits_{\rho_{AB}^o < \rho_A^o + \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o = \int\limits_{\rho_{AB}^o > \rho_A^o + \rho_B} \rho_{AB}^o - \rho_A^o - \rho_B
\end{aligned} \tag{3}$$

As a consequence, we can reformulate $P[\rho_A^o + \rho_B - \rho_{AB}^o]$:

$$\begin{aligned}
P[\rho_A^o + \rho_B - \rho_{AB}^o] =& \frac{1}{2} \cdot \int |\rho_A^o + \rho_B - \rho_{AB}^o| \\
P[\rho_A^o + \rho_B - \rho_{AB}^o] =& \frac{1}{2} \cdot \int\limits_{\rho_{AB}^o < \rho_A^o + \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o + \\
& \frac{1}{2} \cdot \int\limits_{\rho_{AB}^o > \rho_A^o + \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o \\
P[\rho_A^o + \rho_B - \rho_{AB}^o] =& \int\limits_{\rho_{AB}^o < \rho_A^o + \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o.
\end{aligned} \tag{4}$$

We can then split the integration space and obtain:

$$\begin{aligned}
P[\rho_A^o + \rho_B - \rho_{AB}^o] =& \int\limits_{\rho_{AB}^o < \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o + \\
& \int\limits_{\rho_B \leq \rho_{AB}^o < \rho_B + \rho_A^o} \rho_A^o + \rho_B - \rho_{AB}^o.
\end{aligned} \tag{5}$$

Which in turn leads to:

$$P[\rho_A^o + \rho_B - \rho_{AB}^o] = M[\rho_{AB}^o - \rho_B] + \int_{\rho_{AB}^o < \rho_B} \rho_A^o + \int_{\rho_B \leq \rho_{AB}^o < \rho_B + \rho_A^o} \rho_A^o + \rho_B - \rho_{AB}^o. \tag{6}$$

The fact that both integrals on the right hand side of Eq. 6 are non-negative guarantees that:

$$P[\rho_A^o + \rho_B - \rho_{AB}^o] \geq M[\rho_{AB}^o - \rho_B], \tag{7}$$

while the upper bound in Eq. 1 is apparent from Eq. 4.