

Taking out the zero terms and adding up gives

$$E^{Corr} = \frac{1}{2} \sum_{i,j}^{occupied} \sum_{a,b}^{virtual} \frac{|(ia|jb)|^2 + |(ib|ja)|^2 - 2|(ia|jb)(ib|ja)|}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

$$+ \frac{1}{2} \sum_{i,j}^{occupied} \sum_{a,b}^{virtual} \frac{|(ia|jb)|^2}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b} + \frac{1}{2} \sum_{i,j}^{occupied} \sum_{a,b}^{virtual} \frac{|(ib|ja)|^2}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

in which the first line originated from the cases in which the spin for  $i$  and  $j$  was the same (same spin, SS) and the second line came from the last four lines of the previous formula in which the spin for  $i$  and  $j$  was opposite (opposite spin, OS).

The last step is to realize that  $a$  and  $b$  are dummy summation indices that can be renamed to make the second and third summation identical and simplify the first:

$$E^{Corr} = \sum_{i,j}^{occupied} \sum_{a,b}^{virtual} \frac{(ia|jb)\{(ia|jb) - (ib|ja)\}}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

$$+ \sum_{i,j}^{occupied} \sum_{a,b}^{virtual} \frac{(ia|jb)^2}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

the first line (SS) here has a full summation over  $i$  and  $j$ , we can also exclude the terms with  $i=j$  or  $a=b$ , because these are zero (the term in parentheses then cancels out). For the second term (OS), the summation should be over all  $i, j$  and all  $a, b$  including the  $i=j$  and  $a=b$  cases.

Side note: The splitting in SS and OS terms can be used to (empirically) correct for the different errors that are typically found in both contributions. This is the basis for the so-called spin scaled MP2 approach of Grimme and coworkers.

d. Use the above expression to demonstrate the size extensivity of the MP2 energy expression. Hint: assume localized orbitals and consider atoms infinitely far apart so that an integral  $(ia|jb)$  is only non-zero if all orbitals belong to the same atom.