

Figuring out TDDFT shapes

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1 PySCF

TDA excitation vectors are a list of length $\text{nocc} \times \text{nvirt}$; it is clear that each of these corresponds to an excitation energy. However, each element of the list has two entries; the first of which is an ndarray with shape $(\text{nocc}, \text{nvirt})$ and the second of which is just 0. When I move to the RPA, it is similar, but instead of just 0, the second entry is also an ndarray with shape $(\text{nocc}, \text{nvirt})$.

2 Mine

I just have my TDA excitation vectors as an ndarray with shape $(\text{nocc} \times \text{nvirt}, \text{nocc} \times \text{nvirt})$. This is a simplification that needs to change.