STEEPLECHASE FOR 2-RDM APPROXIMATIONS

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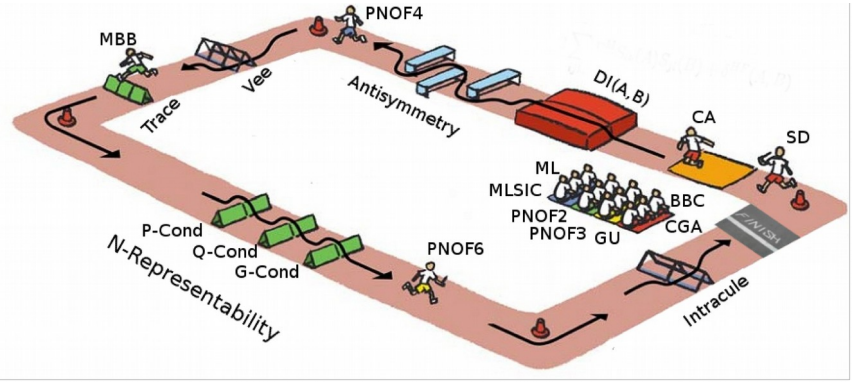
In this work, we will present some tests that we have performed to analize the goodness of second-order reduced density matrices approximations (2-RDM) when the effects of correlation become important. The approximations studied are used to construct functionals in natural orbital functional theory[1-3] .

The battery of tests presented here include: the delocalization index, the calculation of the 2-RDM trace, the termwise error for diagonal elements and for the whole matrix, the fulfillment of some *N-Representability*[2,4] conditions, the attainment of symmetry properties and magnitudes related to the intracule density. Unlike common tests that are based on the reproduction of the electronic energy, this battery of tests offer a wide variety of assessments that permit to check relevant features of the 2-RDM that are normally not put into test.

To tune the correlation effects and dispose of a wide range of correlation regimes, we have chosen the Harmonium atom (HA) model[5] as our reference system. In HA, the effects of correlation are driven by one single parameter called the confinement strength. This model systems provides a realistic description of electron correlation effects and renders itself to analytic solutions for some values of the confinement strength. Harmonium has been used to calibrate DFT functionals[6] and third-order reduced density matrices[7].



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