Construction or Refinement of Approximate Reduced Density Matrices

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One electron density matrices (1RDM) are useful tools since they convey information concerning charge, spin and momentum densities. Their determination from ab-initio calculations is nowadays straightforward for simple systems. However, few attempts have been made to construct a semi-empirical 1RDM from data originating from different experiments [1]. One difficulty is the lack of a generic model, generalizing the Hansen-Coppens approach for charge density refinements. Furthermore, when reaching large systems, such as those encountered in biology or pharmacology, ab-initio methods turn out to be both cumbersome and sometime "too" precise [2].

After a brief review, we will propose, for those two issues, some suggestions and tracks that are or can be fruitfully explored.

[1] Gillet J.M., Becker P., *J.Phys. Chem Solids*, 2004, **65**, 2017. [2] Ragot S, Gillet J.M., Becker P., *Physical Review B,* 2002, **65**, 235115.

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