

A Kohn-Sham-Like Model for the 1-Body Reduced Density Matrix from a Strongly-Correlated Reference

P. A. Johnson¹, P. W. Ayers^{1,*}, S. De Baerdemacker², D. Van Neck³, P. Bultinck⁴

¹ Department of Chemistry and Chemical Biology, McMaster University, L8S 4M1, Hamilton, Ontario, Canada

² Vakgroep Subatomaire-en Stralingsfysica, Universiteit Gent, Proeftuinstraat 86, B-9000 Gent, België

³ Centrum voor Moleculaire Modelling, Universiteit Gent, Technologiepark 903, B-9052, Zwijnaarde, België

⁴ Vakgroep Anorganische en Fysische Chemie, Universiteit Gent, Krijgslaan 281 S3, B-9000 Gent, België

* Corresponding author: ayers@mcmaster.ca

Kohn-Sham density functional theory (KS-DFT)[1] is a very popular and successful approach to approximating the many-body Schrödinger equation due to its favourable speed and moderate accuracy. A non-interacting reference state (Slater determinant) which reproduces the correct electron density is employed. A correction term is then added to connect the fictitious non-interacting system to the real physical system of interest. Unfortunately, this correction term is unknown, and likely unknowable.

The goal of this work is to produce a method in the spirit of the KS approach using the 1-body reduced density matrix (1-RDM) as the fundamental variable rather than the electron density. A strongly-correlated reference state (pairing wavefunction)[2] is employed to achieve this result. Two different approaches to achieve this goal will be presented which are able to treat open- and closed-shell systems. These approaches are able to reproduce both the non-interacting and strongly-correlated limits.

References:

1. Kohn, W. and Sham, L. J. *Phys. Rev.* 140 (1965) A1133.
2. Richardson, R. W. *Phys. Lett.* 3 (1963) 277.