Symbolic algebra development of higher order electron propagator: formulation and implementation

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During the derivation of the electron propagator a perturbative approach is used in order to achieve practical computer implementation. Second and third order propagator methods have been implemented [1-3] in several software packages and its expressions are well known. However, the derivation and the implementation of higher order propagator is very demanding. Some other ab Initio methods have faced a similar problem and have solved it by the development of software packages that automate the algebraic treatment and make the code implementation into computational quantum chemistry software packages through symbolic algebra methods[4].

In this work, a new algorithm to get automatically FORTRAN 90 code for the Quantum Chemistry code LOWDIN has been obtained. This algorithm is based on the use of symbolic algebra treatment of the propagator formulation in order to obtain the self-energy matrix expression to different orders in terms of the electron repulsion integrals and orbital energies. We expect that it will simplify further implementations and help to popularize the use of propagator methods.

[1] J. Linderberg, Y Öhrn, *Propagators in Quantum Chemistry*, Wiley-Interscience, 2 edition, **2004**.

[2] J. V. Ortiz, *Adv. Quantum Chem.* **35**, 33 (1999).

[3] L. S. Cederbaum, W. Domcke, *Adv. Quantum Chem.* **36**, 205 (1977).

[4] So Hirata, *Theor. Chem. Acc.* **116**, 2 (2006).

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