Toward the development of new propagator methods.

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Many-body Green's functions or propagators are powerful tools in the description of electronic structure. Propagators provide a direct path to calculate and interpret differences of energies, electronic properties and Dyson orbitals, with the advantage that the information which can be obtained is not limited to the ground state. Electron propagator methods have shown enormous success in providing practical means of calculating electron binding energies, Dyson orbitals, and ground-state properties from first principles. New approximations based on propagators can be derived through the construction of diagrams or using super-operator theory. Super-operator theory provides a precise, rigorous, consistent and flexible alternative to diagrams for deriving approximations. However, the application of super-operator theory in the derivation of new and more sophisticated propagators can be an overwhelming, non-trivial task. Although there are codes that can be used for the derivation of different electronic structure theories, these codes use several simplifications in the algebra associated with the respective Lie group, limiting the types of approximations than can be derived. In this work, a code for symbolic super-operator manipulation based on functional programming and a variation of an artificial neural network model, often used in machine learning and artificial intelligence, is presented. This code presents a powerful tool in the derivation of not only propagator methods but also any approximation that uses operators corresponding to the Lie unitary subgroup Su_x. As an example of the potential of this tool, we present results related to the derivation of a new electron propagator method in which determinants more general than Hartree-Fock reference determinants are used. This new electron propagator method is intended for the calculation of ionization energies of open shell molecules in which the spin contamination represents a challenge in the calculation of correct and accurate energies.