A brief outlook of the contracted equations formalism and effectiveness of combining the G-particle-hole Hypervirial and the Hermitian-operator methods

C. Valdemoro[1], D. R. Alcoba[2], O. B. Oña[3], L. M. Tel[4], G. E. Massaccesi[5]

[1] Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas, Spain
[2] Departamento de Física, Universidad de Buenos Aires, and Instituto de Física de Buenos Aires, Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina
[3] Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas, Universidad Nacional de La Plata, CCT La Plata, Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina
[4] Departamento de Química Física, Universidad de Salamanca, Salamanca, Spain
[5] Departamento de Ciencias Exactas, Ciclo Básico Común, Universidad de Buenos Aires, Argentina

C. Valdemoro, CSIC, Serrano 123, 28006 Madrid, Spain, c.valdemoro@iff.csic.es

After a brief outlook of the 2-order Contracted Schrödinger and Liouville equations theory[1, 2, 3], we focus our attention on the 2-order G-particle-hole hypervirial (GHV) method[4]. In the GHV method one looks for a 2-order *G-particle-hole* matrix which is a 2-electron quantum average of the Electronic Correlation of the N-electron state considered. Then[5], we show the effectiveness of combining the GHV method with the Hermitian Operator (HO) method of Bouten, Van Leuven, Mihailovich and Rosina[6]. Thus, the G-particle-hole matrix corresponding to a given state of an N-electron system contains all the needed data for applying the HO-method which yields a set of energy values corresponding to the spectrum of the system. A preliminary study of the reduction of the computational cost due to the use of the molecular spatial symmetry is also included. The results obtained with this approach in a series of calculations are presented here.

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