

Some theoretical questions about the G-particle-hole hypervirial equation

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The G-particle-hole hypervirial (GHV) equation^{1,2,3} is the anti-Hermitian part of the second-order Correlation Contracted Schrödinger equation (2-CCSE)⁴. It has been shown that an iterative solution of the GHV equation leads to a very precise description of the electronic structure of an N-electron system. Some theoretical as well as applicative questions are however only partially answered. The aim of this work is to discuss these questions and describe the trends of our present quest in order to optimize further this methodology.

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³ D. R. Alcoba, Phys. Rev. A 65, 032519 (2002).

⁴ D. R. Alcoba, L. M. Tel and E. Pérez-Romero . In preparation