HYLLERAAS-CI CALCULATIONS ON BORON ATOM

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Abstract

The Hylleraas-Configuration Interaction method (Hy-CI) [1-3] combines the inclusion of the interelectronic coordinates in the wave function with the usage of the Configuration Interaction method (CI). The application of the Hylleraas method to light atoms up to Be [4,5] and molecules [6-8] is known to lead to highly accurate energy and properties results. With the development of the computer technology and the accuracy of the experiments, there is a renewed interest in the Hy-CI method. The challenge today is to apply the method to the highly accurate calculation of the second row of atoms and new molecules. For that some mathematical techniques in atomic and molecular calculations have been investigated like the Hamiltonian in Hylleraas coordinates [9], and alternative methods of integral evaluation [10,11] which save computer memory. Boron atom represents well the atoms of the second row, it possesses an angular ground state ^{2}P and s-,p-, and d-orbitals are needed to construct many kinds of symmetry adapted configurations. First CI calculations of B atom have been carried out reproducing the results from other authors [12], in this way a large amount of the correlation energy was included [13]. Afterwards the first Hy-CI calculations on boron atom have been performed [14], the results are very promising. A small number of configurations leads to comparable results to CI calculations using thousands of configurations. We have tested the computer program with He atom for which an energy of nanohartree accuracy was obtained in a time of 130 s [15]. The newest results are reported.

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