RYDBERG AND DOUBLY EXCITED STATES OF THE HELIUM HYDRIDE ION

S. BEZZAOUIA, I. BOUHALI, M. TELMINI, LSAMA, Department of Physics, Faculty of Sciences of Tunis, University of Tunis El Manar 2092 Tunis, Tunisia;
CH. JUNGEN, Department of Physics and Astronomy, University College London, London WC1E 6BT, United Kingdom.

For years, the scientists were interested in the formation/destruction of the helium hydride ion \( \text{HeH}^+ \) which is the first molecular specie appearing in the universe. This molecular ion is present in white dwarfs and intervenes in several molecular processes. Very recently, for the first time, the \( \text{HeH}^+ \) ion was detected outside the laboratory in the planetary nebula NGC 7027 \(^1\). Highly accurate calculations on electronic excited states and rovibronic levels of this system are required to investigate its spectroscopy and dynamics. Several theoretical studies have been devoted to \( \text{HeH}^+ \) and yielded to the determination of excited states of \( \text{HeH}^+ \) for which the principal quantum number \( n \) up to 5. During these last years, our team in Tunis, in collaboration with Dr. Christian Jungen, developed a code to investigate the excited states of diatomic molecules with two active electrons called the \textit{Halfium} code. The first applications of the code focused on hydrogen molecule \( \text{H}_2 \) \(^2\) then on the hydrohelium ion \( \text{HeH}^+ \). For this ion accurate \textit{ab initio} calculations on singly excited electronic states were performed with principal quantum numbers \( n \gg 5 \) \(^3\). Some theoretical studies have been devoted to the evaluation of energy positions and autoionizing widths of doubly excited states of \( \text{HeH}^+ \). We can cite the work of Fernández and Martín \(^4\). They were interested in Q1 and Q2 doubly excited states for \( ^1\Sigma^+ \) and \( ^1\Pi \) symmetries lying respectively above the first and second ionization thresholds. Our work consists in a systematic study of discrete and continuum states of \( \text{HeH}^+ \) using the \textit{halfium} code for various internuclear distances within Born-Oppenheimer approximation. In this contribution, we present our results for singly and doubly excited states for singlet symmetries of \( \text{HeH}^+ \) \(^5\). The obtained potential energies and widths of doubly excited states are compared to other published data.


p-number: p134 Submitted on Fri May 31 11:52:47 CEST 2019