Determination of the adiabatic and nonadiabatic corrections for HeH^+ in Kolos-Wolniewicz basis

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The helium hydride ion (HeH^+) is one of the first particles that emerged after the Big Bang. This molecule along the helium molecular ion were both formed and destroyed on similar pathways during the processes in the early Universe[1,2], which makes them especially interesting from the point of view of astronomical research[3-4].

The similarity of HeH+ in the atomic structure to a hydrogen molecule opens up the a to conduct highly accurate spectroscopic measuraments[5-9] and also to obtain theoretical approximations of rovibrational levels of a similar accuracy. The co-validation of theoretical and spectroscopic results is then necessary. It consists of comparing transitions visible in the spectrum with those theoretically predicted.

To obtain such precise results, we utilize the Kolos-Wolniewicz basis and use the nonadiabatic perturbation theory (NAPT)[10]. Thanks to this, we are able to determine the Born-Oppenheimer (BO) potential and adiabatic and nonadiabatic corrections with the highest possible accuracy.

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