Rovibrational levels of $\text{He}_2^+$

Jacek Komasa$^1$, Krzysztof Pachucki$^2$

$^1$Faculty of Chemistry, A.Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland
$^2$Faculty of Physics, University of Warsaw, Hoża 69, 00-681 Warsaw, Poland

komasa@man.poznan.pl

Dissociation energies of bound rovibrational states of helium dimer cation ($\text{He}_2^+$) in the ground electronic state have been calculated aiming at 0.01 cm$^{-1}$ accuracy. For this purpose all the leading nonadiabatic, relativistic, and quantum electrodynamic effects have been included.

The energy levels have been evaluated perturbationally using an expansion of the energy in powers of the fine structure constant, $\alpha$

$$E = E^{(0)} + \alpha^2 E^{(2)} + \alpha^3 E^{(3)} + \alpha^4 E^{(4)} + \ldots$$

The individual terms of this expansion have been evaluated using exponentially correlated Gaussian wave functions. This methodology has previously been applied to two-electron molecules: $\text{H}_2$, $\text{D}_2$, $\text{HD}$, and $\text{HeH}^+$ [1-4]. An extension to the three-electron systems is presented on the poster.

References: