

Correlated $n^{1,3}S$ states for two-electron atoms in screened potentials

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Synopsis Two-electron atoms in screened and exponential cosine screened Coulomb potentials are studied. We have calculated within a Configuration Interaction approach, the ground and first excited states energies, and other mean values, for H^- , He and Li^+ . We analyze their evolution with the screening parameters, and provide practical fits which allow for a practical and rapid evaluation for plasma applications.

We investigate two-electron atoms placed in a plasma environment, where the three interactions between two particles of charges z_i and z_j placed at a distance r_{ij} can be described by the model potential

$$U_{ij}(r_{ij}) = z_i z_j \frac{e^{-\lambda r_{ij}}}{r_{ij}} \cos(\delta r_{ij}), \quad (1)$$

where λ and δ are positive real parameters. In a weakly coupled plasma the interaction can be described by a Debye-Hückel or screened Coulomb potential (SCP) which corresponds to $\delta = 0$. When the plasma density increases, multi-particle cooperative interaction can be modeled by an exponential cosine screened Coulomb potential (ECSCP) which is given by Eq. (1) with $\lambda = \delta \neq 0$ [1]. For both model potentials the parameter λ is related to the plasma frequency.

Quite recently, Ghoshal and Ho [2] have published the first calculations of the ground states of H^- ($z_3 = 1$) and He ($z_3 = 2$) in a ECSCP on a wide range of screening parameters λ . Highly correlated Hylleraas-type expansions were used. For H^- , mean values $\langle r_{ij}^p \rangle$, with $p \in \mathbb{Z}$, were also provided.

First we wanted to confirm the published results with relatively simpler wave functions. For this purpose, we have used a Configuration Interaction approach with correlated basis functions which explicitly depend on the three inter-particle distances [3, 4, 5, 6]. Each basis function is analytical and consists of the product of two hydrogenic functions multiplied by a distortion factor [3, 4]; it satisfies exactly all two-body Kato cusp conditions [7]. This property is not affected by an appropriate multiplying polynomial [6]. Such a basis has proved quite efficient for a wide range of three-body systems [4, 5].

The main aim of the present investigation is to extend the findings of Ghoshal and Ho in var-

ious directions: (i) we include also the Li^+ ion to observe the expected evolution with the nuclear charge z_3 ; (ii) we evaluate the mean values $\langle r_{ij}^p \rangle$ also for He and Li^+ ; (iii) we provide analytical fits of the energy $E(\lambda)$ and some mean values $\langle r_{ij}^p \rangle(\lambda)$ as a function of λ for both SCP and ECSCP models, i.e. an easy to use tool to estimate the evolution of these quantities with the screening parameter λ ; we further extend the investigation to the iso-electronic series. Considering higher values of z_3 allowed us to provide a double fit $E(\lambda, z_3)$ - this may be of interest for plasma applications; (iv) we make a systematic investigation of the λ_0 value for which the ground state ceases to exist, i.e. $E(\lambda_0) = 0$; (v) we also investigate the evolution with λ of the energy spectrum, by providing the energies of the first $1,3S$ excited states for He and Li^+ .

The evolution of the energy and some mean values $\langle r_{ij}^p \rangle$ as a function of λ for both SCP and ECSCP models for the He atom, and the H^- and Li^+ ions, will be presented at the conference. Analytic fits of the kind $E(\lambda, z_3)$ will also be provided.

References

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