Critical nuclear charge and shape resonances for the two-electron Hamiltonian

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Synopsis We report an improved calculation for the energy of the $2p^2\ ^3P^e$ state of H⁻ and a new determination of the critical nuclear charge Z_{cr} for the $2p^2\ ^3P^e$ state of the two-electron Hamiltonian, using the variational method in Hylleraas coordinates. The achieved precision for the energy and the critical nuclear charge is accurate, respectively, to 29 and 15 significant digits. We further investigate the resonance regime of $Z < Z_{cr}$ using the method of complex scaling.

For H⁻, the energy of its ground state $1s^2\ ^1S^e$ has been accurately determined (see [1, 2, 3] and references therein). The critical value of Z, denoted by Z_{cr}, below which the two-electron ion becomes unbound, has also been determined by several authors with the latest entry in the literature giving 16-digit accuracy [3]. For the region when $Z < Z_{cr}$, the situation becomes more complicate, as the bound state now crosses the ionization threshold and turns into a shape resonance [4 - 6]. As a shape resonance lies in the scattering continuum, we cannot use the usual Rayleigh-Ritz bound principle to optimize its energy. In Refs. [6, 7] the complex resonance energies were determined using the method of complex scaling (see [8] and references therein). For the metastable $2p^2\ ^3P^e$ state in H⁻, the critical value of Z has also been calculated but is only accurate to 3 digits: $Z_{cr} \approx 0.994$, see [9]. Furthermore, the resonance region where $Z < Z_{cr}$ has not been studied before, to the best of our knowledge. In this conference we will report an improved calculation for the bound state energy of $2p^2\ ^3P^e$ of H⁻ and an improved determination of Z_{cr} for the same configuration. The achieved precision for the energy and the critical nuclear charge is accurate to 29 and 15 significant digits, respectively.

The method of complex scaling is used to determine the complex energies of the resonance poles when the metastable bound state turns into a shape resonance when $Z < Z_{cr}$. We use basis set in Hylleraas coordinates to describe the correlations between the two electrons. For the shape resonances we also adopt CI-type bases to check consistence for the resonance energies and widths. Figures 1 and 2 show, respectively, the resonance energy and half-width as a function of $1/Z$.
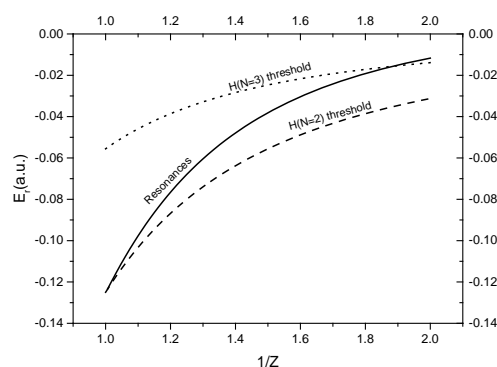
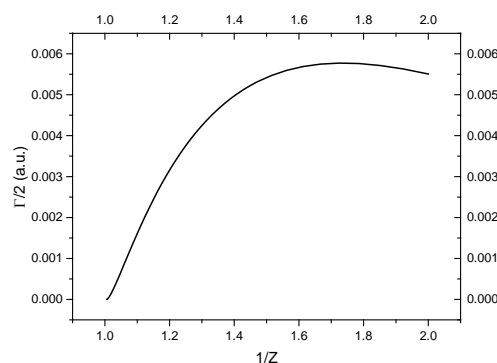**Figure 1.** Resonance energy E vs $1/Z$.

Figure 2. Resonance half-width $\Gamma/2$ vs $1/Z$.

References

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