

B.5.3. Proof of No $^4S^0$ Resonance in H^{2-} --Toru Morishita, C.G. Bao* and C.D. Lin

The question of whether a proton and three electrons can form a bound state or a resonance has fascinated experimentalists and theorists since the 70's. It was not until 1995 that both theory and experiment appear to agree that there are no bound or resonance states in H^{2-} [1-4]. This issue was rekindled in 1996 in a PRL paper by Sommerfeld *et al.*, [5]. In that paper they showed that there is a broad resonance in the $^4S^0$ symmetry. This conclusion is not in contradiction with all the previous works, in principle, since all those works dealt with the $^2P^0$ symmetry. This new finding, which is based on the state-of-the-art quantum chemistry code, is quite surprising to us. Intuitively we believed that the conclusion was incorrect. But we soon realized that we needed to offer a more concrete proof since experimentalists were making plans to search for such a resonance.

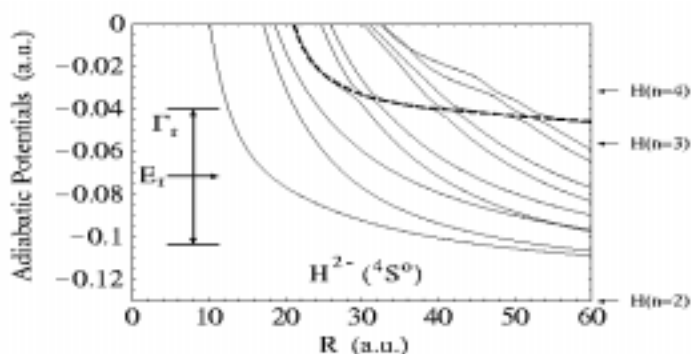


Figure 1. The first few hyperspherical potential curves for $^4S^0$ states of H^{2-} . Also indicated are the energies of the $H(n=2,3,4)$ thresholds. The energy and width of the resonance predicted by Sommerfeld *et al.*, [5] are also indicated (from Publication #102).

We have developed a hyperspherical approach that can calculate the adiabatic potential curves for any three-electron atomic systems [see B.5.2]. These potential curves can provide a first order estimate of the existence of bound states or resonances. In Fig. 1 we show the result from our calculation for the $^4S^0$ symmetry of H^{2-} (Publication #102). The adiabatic potential curves are all repulsive, thus there is no chance for any bound states or resonances to exist. On this figure, the resonance position and width predicted from the calculation of Sommerfeld *et al.* are also shown. The width they predicted is indeed very broad and does not appear to be physical. Using different reasoning, based on the symmetry property of three-electron systems, we argued [see B.5.5] that if there is a resonance in $^4S^0$ symmetry then there should be one in $^2P^0$ symmetry at lower energies. Since no $^2P^0$ resonances were found in the experiment, the $^4S^0$ resonances should not exist.

Since our Publication #102, there has been another paper claiming that H^{2-} has two $^4S^o$ resonances [6]. This work was supposed to be an improved calculation using a computational method similar to the one used by Sommerfeld *et al.*, [5]. Experimentally, electron impact on B^- ($1s^2 2s^2 2p^2 \ ^3P^e$), in principle, can produce $^4S^o$ resonances if they exist, but no resonances have been observed [7]. This serves as an indirect experimental proof of no such $^4S^o$ resonances.

References

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