B.5.2. Hyperspherical Approach for Three-Electron Atoms--*Toru Morishita and C.D. Lin*

In the last period we have refined the computational methods for carrying out calculations on three-electron atoms in hyperspherical coordinates. The details can be found in Publication #100. In this method the radial distances r_1, r_2, and r_3 are replaced by a hyperradius R and two hyperangles α_1 and α_2,

$$\begin{aligned} r_1 &= R\sin\alpha_2\cos\alpha_1, \\ r_2 &= R\sin\alpha_2\sin\alpha_1, \\ r_3 &= R\cos\alpha_2 \end{aligned} \tag{1}$$

By treating the hyperradius R as an adiabatic parameter, we rewrite the Schrödinger equation as

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial R^2} + H_{\mathrm{ad}}(\Omega;R) - E\right]\psi = 0\,, \tag{2}$$

where the solution at fixed R satisfies

$$\left[H_{\mathrm{ad}}(\Omega;R) - U_\mu(R)\right]\Phi_\mu(\Omega;R) = 0\,. \tag{3}$$

The total wavefunction is expanded as

$$\psi^s = \sum_\mu F_\mu^s(R)\left(\sum_{S_{12}} \Phi_\mu^{S,S_{12}}(\Omega;\mathrm{R})\,\chi_{S_{12}}^S\right). \tag{4}$$

The function Φ_μ is the adiabatic channel function and χ is the total spin function. From solving the Hamiltonian with a fixed R, a family of potential curves is obtained. Details of the computational method are discussed in Publication #100. The main point is that we now have an efficient method for solving the hyperspherical potential curves and the associated wave-functions, for any three-electron systems, and for any symmetries characterized by L, S and π, the total orbital and spin angular momentum, and parity, respectively. The solutions include not only singly excited states, but also doubly excited states and triply excited states.

As an example, in Fig. 1 we show the family of potential curves for $^2S^e$ states of Li. The lowest curve goes to the $1s^2\ ^1S^e$ limit of Li^+ at large R. Therefore the ground state and the $1s^2ns$ $^2S^e$ singly excited states are the bound states supported by this lowest curve.

The next group of potential curves supports doubly excited states. By focusing on the lowest few of these curves, as shown in Fig. 2, and comparing with the corresponding set of potential curves of He, one can immediately recognize that the two sets of curves are very similar. This shows that the classification scheme for the doubly excited states of two-electron atoms that we have developed previously [1] can be used to classify doubly excited states of a three-electron atom. The correlation of the two excited electrons depends little on the existence of the core electron. Figure 2 also reveals that the potential curves in the asymptotic region are different due to the splitting of the 1s2s $^{1,3}S^e$ and 1s2p$^{1,3}P^o$ states of Li$^+$ as compared to the degenerate 2s and 2p states of He$^+$. Such difference results in more complicated spectroscopy for the doubly excited states of Li.

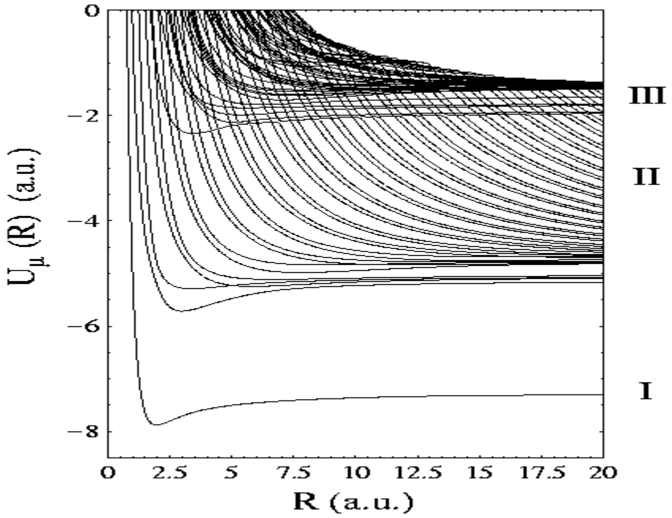

Figure 1. Hyperspherical potential curves for $^2S^e$ states of Li. The lowest curve labeled I supports singly excited states of Li. The group of curves labeled II support 1snℓn'ℓ doubly excited states. The group labeled III support triply excited states (from Publication #100).

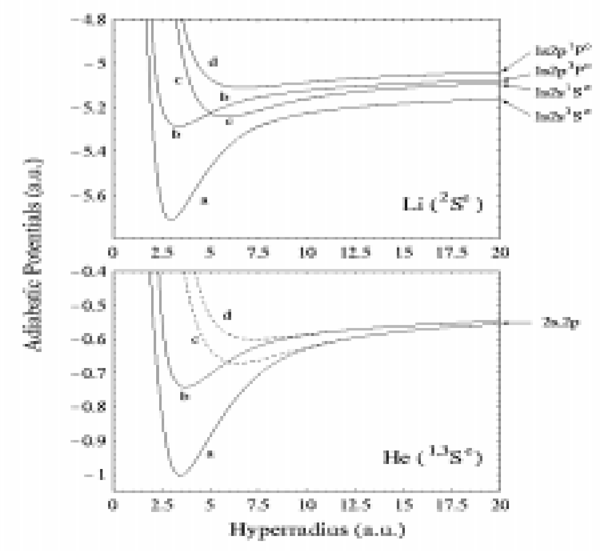

Figure 2. Comparison of hyperspherical potential curves for the 1s2ℓnℓ $^2S^e$ doubly excited states of Li with the 1snℓ $^{1,3}S^e$ doubly excited states of He. The similarity of the potential curves at small R implies that the new classification quantum numbers K, T and A for describing doubly excited states of He can be used to describe doubly excited states of Li (from Publication #100).

Reference

1. C.D. Lin, Phys. Rev. A 29, 1019 (1984).