POSITRONIUM IMPACT ON LITHIUM

S Sahoo*, S Gilmore[†] and H R J Walters[†]

*Atomistic Simulation Center, School of Mathematics and Physics, Queen's University, Belfast BT7

1NN, UK

[†]Department of Applied Mathematics and Theoretical Physics, Queen's University, Belfast BT7

1NN, UK

We investigate positronium (Ps) scattering by lithium (Li) using a coupled pseudostate approximation and a model potential one - electron description of the Li atom. The collisional wave function, Ψ , is expanded as

$$\Psi = \sum_{a,b} \left[G_{ab}(\mathbf{R}_1) \phi_a(\mathbf{t}_1) \psi_b(\mathbf{r}_2) + (-1)^{S_e} G_{ab}(\mathbf{R}_2) \phi_a(\mathbf{t}_2) \psi_b(\mathbf{r}_1) \right]$$
(1)

where $\mathbf{r_p}(\mathbf{r_i})$ is the position vector of the positron (ith electron) relative to the Li nucleus, $\mathbf{R_i} = (\mathbf{r_p} + \mathbf{r_i})/2$, $\mathbf{t_i} = \mathbf{r_p} - \mathbf{r_i}$, the sum in (1) is over Ps states ϕ_a and Li valence orbital states ψ_b , and S_e (=0, 1) is the total electronic spin of the system.

The valence states of Li have been generated using the model potential of Stein [1]. We are interested in collisions involving 2s and 2p states of Li. However, the potential of Stein also supports an unphysical 1s state. We have found that omission of this state in the approximation (1) can lead to pronounced unphysical structures in the physical Ps - Li cross sections. Accordingly, we include all three Li states, 1s, 2s, 2p, in (1). We would expect this to give reasonable results provided that cross sections between the physical 2s and 2p states and the unphysical 1s state are small, which they are.

For the Ps states in (1) we have used a nine element set, 1s, 2s, $\overline{3s}$, $\overline{4s}$, 2p, $\overline{3p}$, $\overline{4p}$, $\overline{3d}$, $\overline{4d}$ where states denoted by a 'bar' are pseudostates.

The pseudostates help us to represent the ionization of Ps in a discrete way. Substituting (1) into the Schrodinger equation and projecting with $\phi_a(\mathbf{t_1})\psi_b(\mathbf{r_2})$ leads to coupled equations for the functions $G_{ab}(\mathbf{R})$. These have been reduced to partial wave form and solved using the R- matrix technique.



Figure 1

Figure 1 shows what happens to the Ps irrespective of the final state of the Li atom.

More detailed results will be presented at the Conference.

References

[1] P. M. Stein, J. Phys. B **26** 2087 (1993).