Scientific Report

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1 Purpose of the visit

Professor Tennyson with his group deals with the R-matrix theory of electron-molecule collisions. Recently, the molecular R-matrix method with pseudostates (MRMPS) was developed (Gorfinkiel & Tennyson 2005) and successfully used for calculation of ionisation cross sections by electron impact. An additional property of this method is its ability to represent the polarisability of the target ground state better than it is possible in standard calculations based on the close-coupling expansion of the wave function (Gil et al. 1994).

I am dealing with collisions of electrons with the Li_2 molecule at low energies (Tarana et al. 2008). Li_2 is a diatomic molecule with the largest known static dipole polarisability (Mérawa & Rérat 2001) as well as largest known electron scattering cross sections at low-energies (Gil et al. 1993). Calculation of the electron scattering off this molecule is complicated by the presence of low-lying target excited states.

The main aim of my visit was to calculate the cross sections of the elastic scattering and of the electronic excitation using the MRMPS method and to demonstrate its advantages in representation of the target polarisability. The Li_2 molecule represents a benchmark system for theoretical methods treating the electron scattering off molecules with large polarisability.

2 Work carried out

Due to the large spatial extent of the Li_2 wave function, rather large R-matrix sphere radius (r_Ω=18 a_0) was used. As a consequence, the scattering energy interval studied was restricted to 0-4.5 eV range. This required optimisation of new continuum basis set based on the previously used basis (Tarana et al. 2008) and augmented by higher partial waves. This GTO continuum basis set was tested by performing calculations in the static exchange approximation. We also wanted to obtain pseudostates basis that enables good representation of the target ground state polarisability and which gives energies of the low-lying pseudostates close to the physical target states energies.

The calculations using two different PC bases were performed as well as calculation not using pseudostates. The results were compared in order to understand effects of polarisation as well as to control the stability of the calculations with respect to small change of the PC-basis.

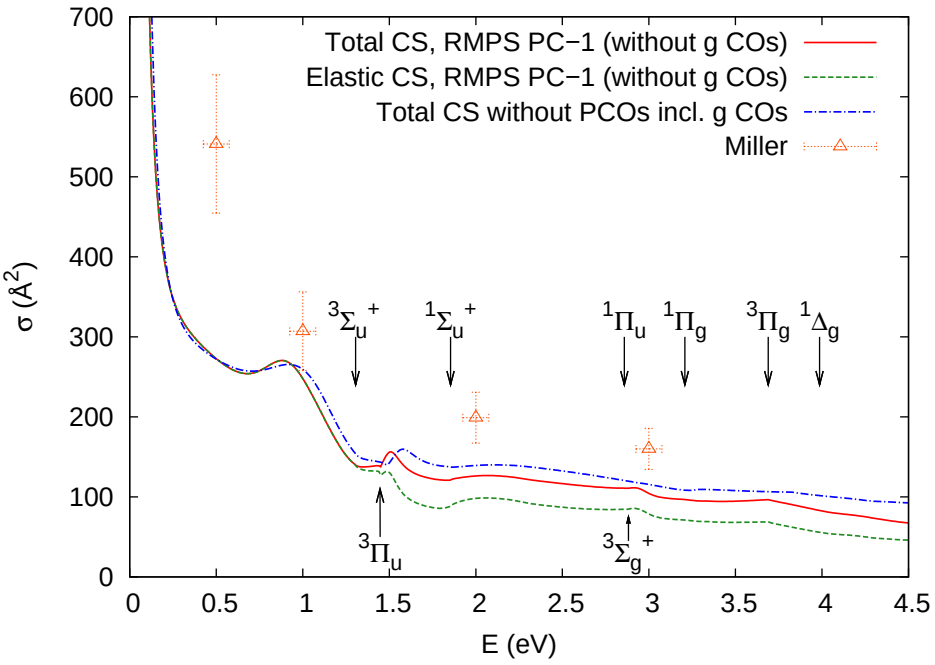
All the calculations were performed using the UK polyatomic R-matrix program (Morgan et al. 1997) in the D_{2h} point group. We calculated the eigenphases and cross sections of the elastic scattering as well as of the electronic excitation. There is a rich resonance structure in the energy interval of our interest. Parameters of several resonances were determined by fitting to the Breit-Wigner formula.

3 Results

Using only a few pseudostates we are able to treat the polarisability of the target ground state in more consistent way than previous studies (Gil et al. 1993, Padial 1985) and represent the low-lying target states correctly.

In general, our cross sections calculated using the MRMPS method are in good agreement with calculations without pseudostates (Figure 1). The elastic scattering cross sections calculated using

Figure 1: Total (elastic plus electronic excitation) cross section calculated using the PC-1 basis. Experimental data due to Miller *et al.* is given by triangles with errorbars.



different pseudocontinuum models show that our calculation is stable with respect to small change of the pseudostates basis. The calculated eigenphases are in good agreement for low-energies, while in the energy region above 2 eV the difference between various calculations starts to be more significant (Figure 2).

The low-lying $^2\Pi_u$ shape resonance reported in previous works (Padial 1985, Gil et al. 1993) is confirmed by our calculations, where it was found at energy about 0.05 eV. Several other low-lying resonances and resonance-like structures were identified as well, although determination of their parameters was complicated by the density of low-lying target states.

Our work appears to be the first *ab initio* calculation of electron collisions with the Li_2 molecule at energies above 1 eV which includes excited states and thus allows for electronically inelastic processes.

4 Publications

The results obtained during my stay are presented in publication prepared very recently and submitted to J. Phys. B: At. Mol. Opt. Phys.

References

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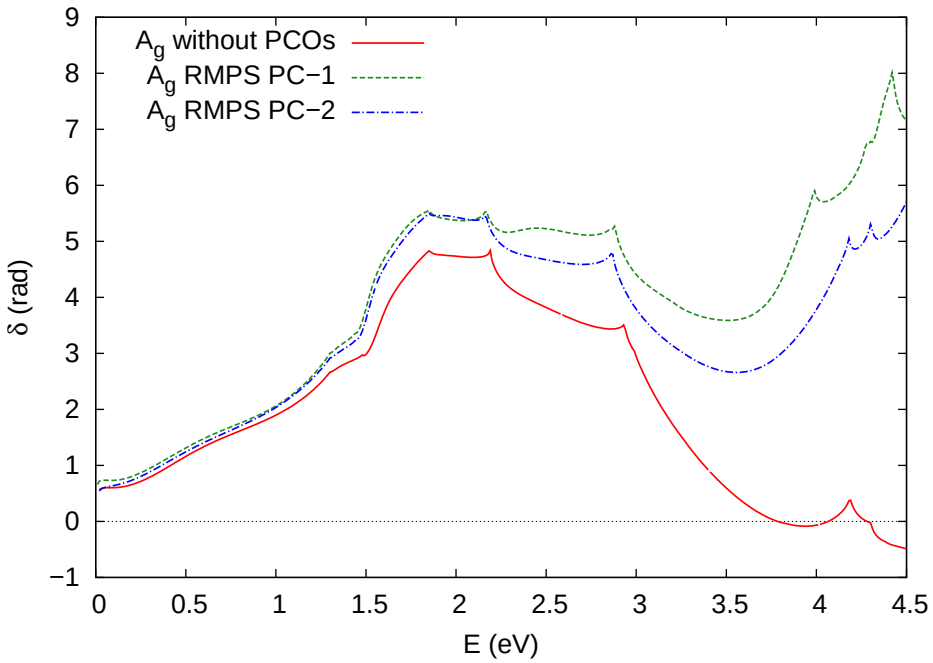
Figure 2: ^2A_g symmetry eigenphase sums as a function of model.



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