MALAYSIAN SCIENCE & TECHNOLOGY CONGRESS '99
Symposium A: Agriculture, Biology, Marine, Medicine, Social Science, Basic Sciences.
25-27 October, 1999. Kuala Lumpur

Optical Potential Study of Positron Scattering by Hydrogenic-type Atoms

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ABSTRACT

An optical potential method based on the close-coupling formalism has been implemented to study positron scattering by hydrogenic-type atoms. The present work will be reviewed in the context of other theories. Preliminary results will be presented and compared with experimental results.

1. Introduction

In the 90's,we have seen major advances in the theoretical studies of positron scattering by atoms. These theoretical studies [1-3] have mainly centred on positron-hydrogen atom scattering process at low energies. These new generation scattering methods provide the most realistic investigations for positron scattering by atomic system as they explicitly couple the positronium (Ps) channels together with the hydrogen atom channels in their theoretical calculations. Concerted efforts by various researchers in the field has culminated in a series of accurate total cross sections for transitions studied at low energies for positron-hydrogen atom system [4-6]. The efforts for other hydrogenic-type atoms have been slow in comparison [7-8].

In recent years, theoretical studies on positron-atom scattering are being focused in the intermediate-energy regime. This is a tremendous challenge, as it would imply a lot of discrete states and the continuum must be incorporated in a practical manner for any theoretical calculations. A simple 6-state close-coupling calculation [9] which allowed 3 H states (1s,2s,2p) and 3 Ps states (1s,2s,2p) to study positron scattering from atomic hydrogen at intermediate energies of 4 – 100 Ryd had been done This work provided a comprehensive and realistic study of the scattering process but nevertheless not complete as higher discrete states and the continuum were neglected. Recently [10,11] had used a large L^2 basis of hydrogen states (30 and 28 states respectively) together with the Ps(1s), Ps(2s) and Ps(2p) states to study positron scattering by atomic H at intermediate energies. Their results provide a useful benchmark for theoretical calculations in the intermediate energy region. Nevertheless, there are obvious differences between these two studies. This motivated the most recent work of Ratnavelu and Rajagopal [12] that implemented the coupled-channels-optical method (CCOM) for the positron-hydrogen atom scattering.

In this work, we report our efforts to demonstrate the optical potential method to study positron-hydrogen scattering and positron-sodium scattering systems. Due to constraints here, we will not provide all the theoretical details but focus in the general development of the optical potential formalism.

2. Optical Potential Formalism

The optical potential model has been incorporated within the close-coupling method of Mitroy [1] that allows both manifolds of positron-hydrogen and positronium-proton channels. In the coupled-channels expansion, the total wavefunction is expanded as

$$\Psi(r_1, r_2) = \sum_{\alpha} \psi_{\alpha}(r_1) F_{\alpha}(r_2) + \sum_{\beta} \phi_{\beta}(\rho) G_{\beta}(R) \qquad (1)$$

where $\psi_{\alpha}(r_1)$ are the hydrogenic target states and $\phi_{\beta}(\rho)$ are the positronium states. In implementing the CCOM method, we partition the target space by using the projection operators P and Q where

$$P = \sum_{i \in P} |\psi_i\rangle\langle\psi_i| \qquad (2)$$

and

$$Q = 1 - P \qquad (3)$$

Thus, the optical potential $V^{(Q)}$ can be formulated [13], with the Q-space eliminated for the positron-hydrogen channels as

$$V^{(Q)} = V + V\,Q\frac{1}{Q(E^{(+)} - K - K)Q}Q\,V \qquad (4)$$

where $V = v_1 + v_2 + v_3$ with v_1 is the electron-nucleus potential, v_2 is the positron-nucleus potential and v_3 the positron-electron Coulomb potential. The last term in (4) is the complex polarisation potential.

Following McCarthy and Stelbovics [13-14], the complex polarisation term of equation (4) can be calculated. In the present work the Q-space considered only includes the continuum channels. The details of calculating the complex polarisation potential for the continuum can be found in McCarthy and Stelbovics [14] and Ratnavelu [15]. Thus the momentum space Lippmann-Schwinger equations (for a positron with momentum k incident on hydrogen atom in state Ψ_α (atomic units are assumed throughout) can be solved [12].

3. Positron-hydrogen atom scattering

The following calculations were done:

CC(3,3): In this calculation, the simplest model of 3 hydrogen states H(1s), H(2s) and H(2p) and the 3 positronium states Ps(1s), Ps(2s) and Ps(2p) were used.

CCO(3,3): Besides the 6 physical states incorporated in the above close-coupling expansion, optical potentials for the continuum were used in the 1s-1s, 1s-2s, 2s-2s, 1s-2p, 2p-2p and 2s-2p couplings.

CC(6,3): In this model, the six hydrogen states 1s,2s,2p,3s,3p,3d have been included together with the Ps 1s,2s,2p,3s,3p and 3d.

CCO(6,3): This calculation allows for the continuum optical potential in the 1s-1s, 1s-2s,1s-2p,2s-2s,2p-2p and 2s-2p couplings in the 9-state calculation.

The numerical details of solving the coupled Lippmann-Schwinger equations for positron-hydrogen scattering have been well-detailed [1,9,10].

Here we present only the ionisation and Ps formation cross sections. In Figure 1, we show the ionisation cross sections calculated with the CCO(3,3) and CCO(6,3) together with the CC($\overline{28}$,3) and CC($\overline{30}$,3) models. We also depict the ionisation cross section of Ratnavelu [15]. The present CCO(3,3) and CCO(6,3) confirm the qualitative and quantitative features of the continuum optical potential of Ratnavelu. This provides an indirect test that the continuum optical potential has been accurately incorporated in the present work. The present models also show excellent agreement with the UCL data [16] from 30 eV onwards. But the lack of convergence of the L^2 calculations also suggest that further convergence studies must be done to explain the quantitative differences that exist between these two calculations at other intermediate energies. Our calculations demonstrates that the CCO(3,3) and CCO(6,3) have converged over most of the energies. The inevitable question is now to reduce the experimental errors so as to provide a more discriminating test for theories. In Figure 2, the Ps formation cross sections are calculated in the various theoretical approaches and are depicted with the experimental data of the Bielefeld-Brookhaven

collaboration [17] and the Detroit group [18]. We only depict the 'best' measurements of Zhou *et al* [18] and not their lower limit values. The qualitative shapes are reproduced by all theories and there is good quantitative agreement.

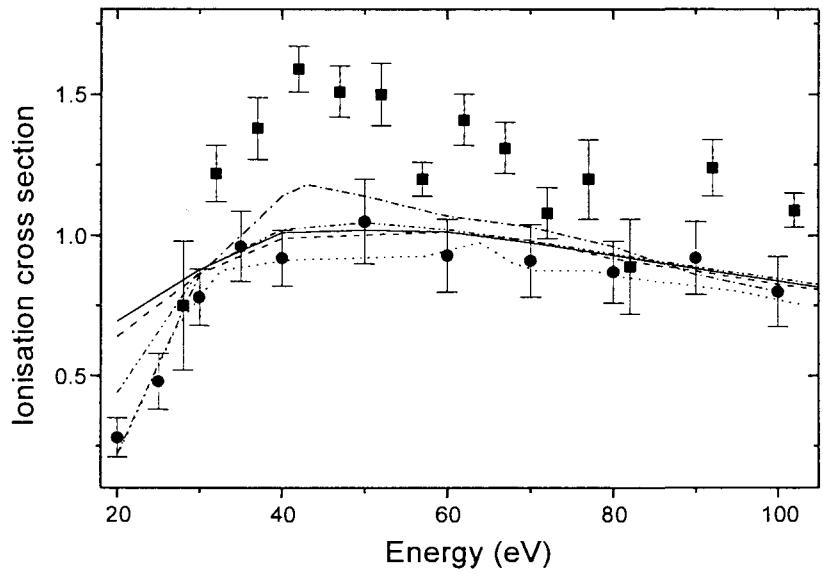

FIGURE 1: The Ionisation Cross Sections (in πa_0^2) for Positron-Hydrogen Scattering: The CCO(6,3) (–), CCO(3,3) (---), Continuum model (-..-), CC($\overline{30}$,3) (-.-), CC($\overline{28}$,3) (...), UCL data (●) and the Bielefeld data (▮).

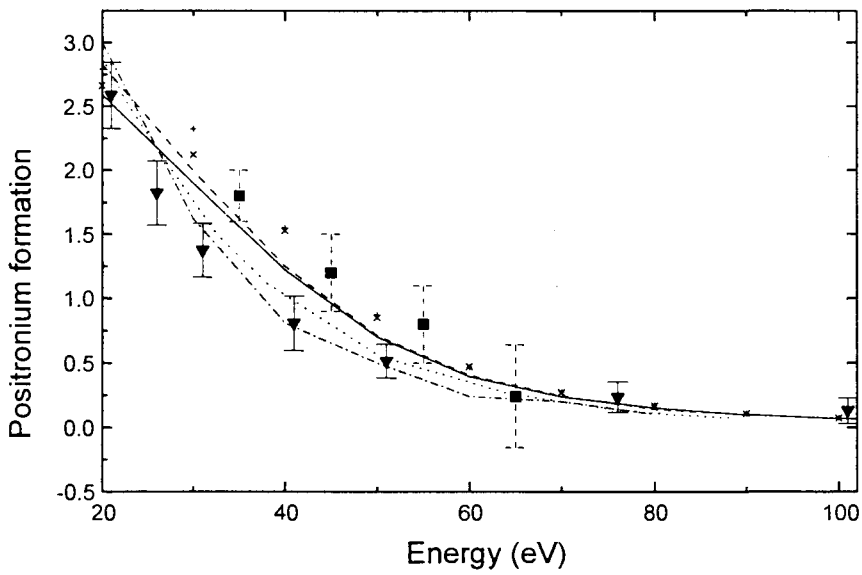

FIGURE 2: The Ps Formation Cross Sections (in πa_0^2) for Positron-Hydrogen Scattering. The Legend for the Theoretical Models are the Same as in Figure 1 except for the CC(3,3) (+) and CC(6,3) (x). The Experimental Datas are from Detroit (▼) and Bielefeld-Brookhaven (■).

4. Positron-Sodium Scattering

Positron-sodium scattering is in actual fact, a many-body problem. However, it can be simplified into a 3-body problem i.e. the incoming positron, the valence electron and the core with the following approximations. Only the valence electron is scattered by the positron. Exchange of core electrons and the valence electron is neglected. Ps formation only involves the valence electron. With these assumptions, the scattering problem becomes very similar to the positron-hydrogen scattering problem.

The following calculations have been done for positron-sodium scattering.

CC(2,3) : The close-coupling calculation using the 2 lowest lying discrete states (3s,3p) and three Ps states i.e. Ps(1s), Ps(2s) and Ps(2p).

CCO(2,3): This is calculation is similar to the CC(2,3) but with an addition of (3s-3s), (3p-3p) and (3s-3p) optical potentials.

Here we present only the Total and Ps formation cross sections. In Figure 3, we show the total cross sections calculated with the CC(2,3) and CCO(2,3) together with the CC(5,3) and the CC(5,6) models. We have also included the experimental measurements of Kwan *et al* [19] for comparison. Overall, the qualitative shape of all the calculations match the measurements.

In Figure 4, we present the Ps formation cross section for positron-sodium scattering using CC(2,3), CCO(2,3), CC(5,3) and CC(5,6). All calculations are observed to underestimate the Ps formation cross section experimental measurements of Stein *et al* [20].

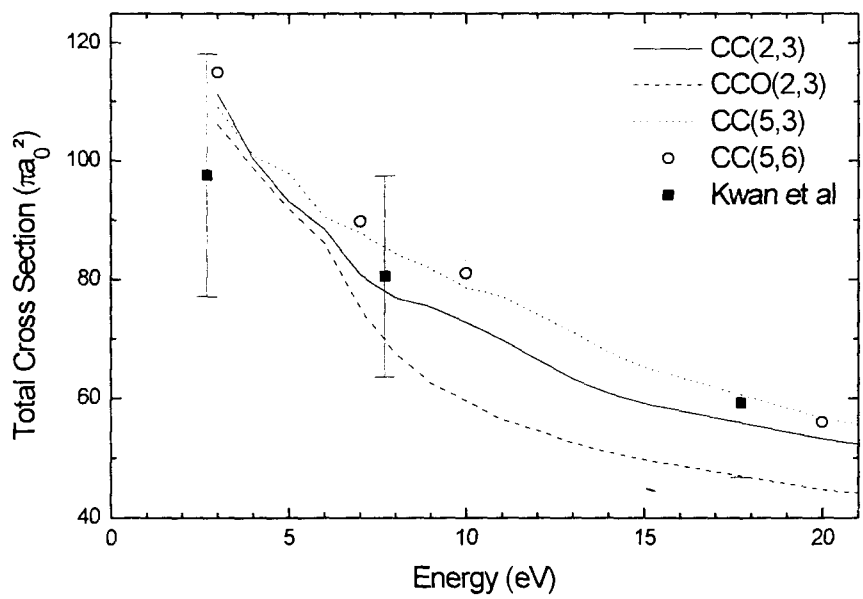

Figure 3: Total Cross Section for Positron-Sodium Scattering

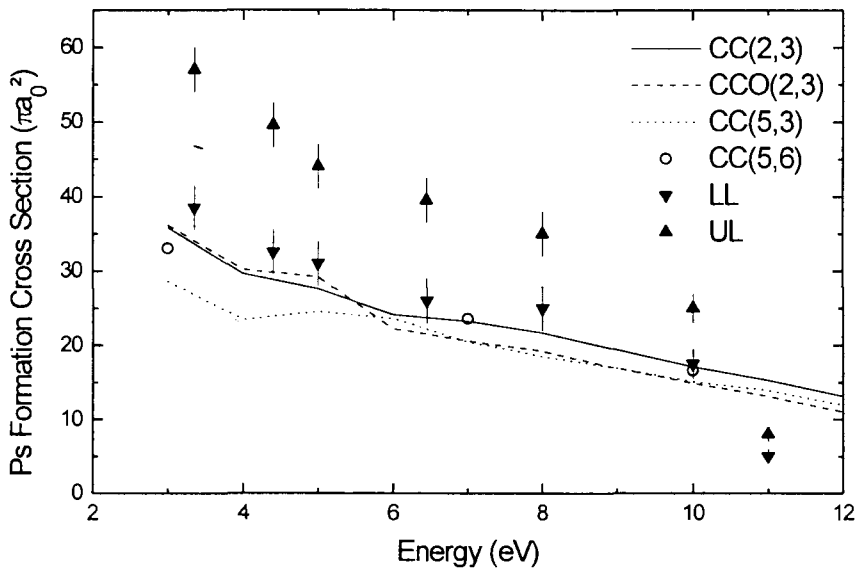

Figure 4: Ps Formation Cross Section for Positron-Sodium Scattering

5. Conclusions

We have reported preliminary work on positron scattering by atomic hydrogen and atomic sodium at intermediate energies using the coupled-channel-optical method. In comparing our results with other theories and experimental results, we are certain that the CCOM has been successfully extended to perform realistic studies of positron scattering from hydrogenic-type atoms.

Acknowledgments

Kuru Ratnavelu would like to thank Dr. Jim Mitroy for the use of his close-coupling code. He also acknowledges the encouragement and support given by Prof. Ian McCarthy. The financial support of the Malaysian Ministry of Science, Technology and Environment under the IRPA Project No: 09-02-03-0382 is gratefully acknowledged.

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