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Positron helium scattering using CCA

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Abstract : Calculations have been carried out to investigate e^+-He scattering using close coupling method with various basis sets The $n = 2$ excitation cross section and positronium cross section are reported at medium energies Two dynamically active electrons have been considered on same footing and realistic wavefunctions of helium target have been used

Keywords : Positron, helium atom, close coupling approximation

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1. Introduction

The positron-helium system is experimentally the most studied one of all the positron-atom systems. This has stimulated theoreticians to investigate the system. Moreover, this problem is very challenging theoretically. This system has all the complications of a many-body problem, but two-body techniques can be employed. The validity and suitability of an approximate model can be tested for this system as measured data are available and will be of great help in solving the more complex situation where accurate calculation is not possible.

At low energy, Humberston [1] and Campeanu and Humberston [2] have reported s wave phase shift using variational method. Campeanu and Humberston [3] and Campeanu [4] have calculated *p*- and *d*-wave phase shifts variationally. These results are expected to be very accurate. The presence of these results will give impetus to theoretical workers to study the system. Apart from these investigations, there are a good number of theoretical calculations found in the literature. Here, we mention some of the investigations that have been carried out using eigenstate expansion method or close coupling approximation (CCA). Willis *et al* [5] and Willis and McDowell [6] have employed single-channel CCA to investigate positron-helium scattering using different basis sets. Mandal *et al* [7,8] have employed a coupled state method to study the same problem. Recently, a two-channel version of CCA was employed by Hewitt *et al* [9] using a 8-state basis : He ($1s$, $2s$, $K\bar{s}$ $2p$, $K\bar{p}$), Ps ($1s$, $2s$, $2p$). An independent electron model with a model potential is used to represent the helium target. In other words, they have assumed a one-electron common central field approximation.

The CCA provides a practical framework for treating electron-atom and positron-atom scattering which can, in principle, be improved upon by including more states of the subsystem in the expansion basis. The two-channel version of CCA handles direct and rearrangement process in an unified way. The necessity of using the two-channel CCA has been emphasised by Basu *et al* [10], Sarkar *et al* [11] and Kernoghan *et al* [12]. It has also been noticed that two-channel CCA is found to be suitable with proper basis set [12] to study positron-atom scattering.

2. Theory

We consider positron helium scattering at low and medium energies using a two channel version of CCA. We consider two dynamically active electrons on same footing and employ realistic wavefunctions of helium target. In the present study, we use the following basis sets :

(A) He ($1s^2$)

(B) He ($1s^2$, $1s\,2^1s$)

(C) He ($1s^2$, $1s\,2^1s$, $1s\,2^1P$)

(D) He ($1s^2$), Ps ($1s$)

(E) He ($1s^2$, $1s\,2^1s$, $1s\,2^1P$), Ps ($1s$).

The reason for using 5 basis sets is to find the relative importance of each state in predicting scattering parameters. Preliminary results of this investigation have been reported by Kahali *et al* [13].

We take the incident positron to be particle 1 and the atomic electrons to be particles 2 and 3 respectively. Assuming the helium nucleus to be infinitely heavy and the centre of the coordinate system, the total wavefunction of the positron-helium system may may be expressed as

$$\Psi(r_1, r_2, r_3) = \sum_n \Psi_n(r_2, r_3) F_n(r_1) \chi_1(1, 23) + \sum_v \Big[\phi_0(r_3) \omega_v(r_{12}) \times \left\{ G_v^P(S_{12})\, \chi_1(3, 12) + G_v^0(S_{12})\, \chi_2(3, 21) \right\} + \phi_0(r_2) \omega_v(r_{13}) \left\{ G^P(S_{13})\, \chi_1(2, 13) - G_v^0(S_{13})\, \chi_2(2, 31) \right\} \Big].$$

where χ_1 and χ_2 are the appropriate spin functions, ψ_n is the wavefunction of helium atom and ϕ_0 stands for ionized helium in the ground state. The wavefunction of Ps atom is denoted by ω_v. F_n describes the motion of the positron and G_v^P and G_v^0 the motion of the Ps atom in the para- and ortho-state respectively, relative to the helium target.

It has been shown explicitly by Mandal *et al* [7] that positron spin does not play any part. The capture probability of a positron by an atomic electron in the ortho-state is three times that in the para-state so that $G_v^0 = \sqrt{3}\, G_v^P$. Summing these two probabilities we obtain the integral equations for the transition amplitude in the momentum space as

$$\left\langle K'n'_\beta \middle| Y_{\beta\alpha} \middle| K1s_\alpha \right\rangle = \left\langle K'n'_\beta \middle| B_{\beta\alpha} \middle| Ks_\alpha \right\rangle + \sum_\gamma \sum_{n''} \frac{\left\langle K'n'_\beta \middle| B_{\beta\alpha} \middle| K''n''_\gamma \right\rangle \left\langle K''n''_\beta \middle| Y_{\gamma\alpha} \middle| K_{1s} \right\rangle}{E - E_{n''}}$$

Here, α or β stands for the channel and n_α is the bound subsystem in the channel α.

Following Mandal *et al* [7,8] and Basu *et al* [10], we obtain coupled integral equations for scattering amplitude and after the partial wave analysis, one dimensional coupled integral equation is formed and the resulting equations may be written as

$$T^J_{\beta\alpha}\left(\tau'_\beta K', \tau_\alpha K\right) = B^J_{\beta\alpha}\left(\tau'_\beta K', \tau_\alpha K\right) + \frac{1}{2\pi^2} \sum_\gamma \sum_{n''} \int \frac{K''^2 dK'' B^J_{\beta\gamma}\left(\tau'_\beta K', \tau''_\gamma K''\right) J_\gamma\left(\tau''_\gamma K'', \tau_\alpha K''\right)}{K''^2 - K^2_\gamma - i\varepsilon},$$

where $\tau_\alpha = (n_\alpha\ lLJ)$. Here, J is the good quantum number and l and L is the angular momentum of the bound subsystem and the incident positron in the channel α respectively. The following helium wavefuctions have been used in the present calculation [14–16] :

$$\phi_{1s1s}(r_1, r_2) = u_{1s}(r_1)\, u_{1s}(r_2),$$

$$\phi_{1s2's}(r_1, r_2) = N\left[u^+_{1s}(r_1)\, v_{2s}(r_2) + u^+_{1s}(r_2)\, v_{2s}(r_1)\right]$$

$$\phi_{1s2'p_m}(r_1 r_2) = N'\left[u^+_{1s}(r_1) v_{2p_m}(r_2) + u^+_{1s}(r_2) v_{2p_m}(r_1)\right],$$

where the atomic orbitals are given by

$$u_{1s}(r) = (1/4\pi)^{1/2} \sum_{i=1}^{2} a_i \exp(\lambda_i r) Y_{00}(\hat{r}),$$

$$u^+_{1s}(r) = \exp(-Zr) Y_{00}(\hat{r}),$$

$$v_{2s}(r) = \sum_{i=1}^{2} B_i r^{i-1} \exp(-\beta_i r) Y_{00}(\hat{r})$$

$$v_{2p_m}(r) = r \exp(-0.5 Z_0 r) Y_{1m}(\hat{r}),$$

with $\lambda_1 = 1.41$, $\lambda_2 = 2.61$, $a_1 = 2.60505$ $a_2 = 2.08144$, $B_1 = 1.0$, $B_2 = -0.432784$, $N = 0.1966184$, $\beta_1 = 0.865$, $\beta_2 = 0.522$, $Z = 2$, $Z_0 = 0.97$ and $N' = \left(Z_0^5/6\pi\right)^{1/2}$.

3. Results and discussion

Kahali *et al* [13] reported *s*-, *p*- and *d*-wave phase shifts below the Ps-formation threshold. It has been found that with the added eigenstates, the phase shift is tending to correct value as expected. However, the rate of convergence is slow compared to electron case. A resonance has been reported in the *s*-wave ground state capture cross section. The total cross section has also been compared with measured data. Here, we present some more scattering parameters of interest.

Figure 1 represents the present 4-state integrated elastic cross sections in the energy range 30–100 eV. The five-state single channel CCA results of Willis and McDowell (WM) [6] and two channel 8-state CCA predictions of Hewitt *et al* (HNB) [9] are compared with those of ours The results of HNB are always less than the present predictions and those of WM in the energy range considered. Hewitt *et al* [9] have adopted an independent electron model for the helium atom. However, they have employed different basis set from that of ours These may be the probable reasons for the difference in results. The present elastic cross sections differ from those of WM in the energy range considered, the predictions of WM being lower. The inclusion of capture in our calculations is expected to make this difference. With the increase of energy, the effect of Ps formation channel on the elastic cross section reduces. This is also evident from the present predictions and those of WM The present result approaches that of WM with the increase of energy and around the incident energy 150 eV (not shown), the two results coalesce.

The $n = 2$ excitation cross section is measured by Sueoka as quoted by Charlton and Laricchia [17] in the energy range 22–100 eV using the time-of flight (TOF) spectra of the scattered positron. In Figure 2. the present $n = 2$ excitation cross sections are compared with measured data of Sueoka. The 8-state results of Hewitt *et al* (HNB) are also given in the same figure Beyond 35 eV, the method has overestimated the excitation cross section when compared with measured data. The predictions of HNB differ from us appreciably beyond the incident energy 40 eV, their results being higher and further away from measured data.

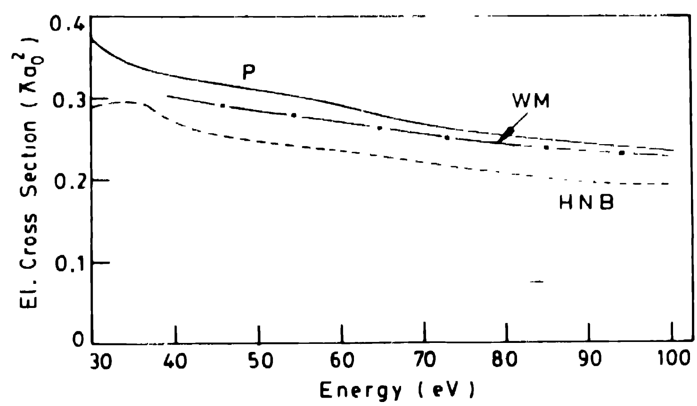

Figure 1. Elastic cross section energy graph. P–Present , WM–Willis and McDowell [6] ; HNB–Hewitt *et al* [9].

It may be mentioned that present $n = 2$ excitation results are very close to those of the first Born results beyond 80 eV.

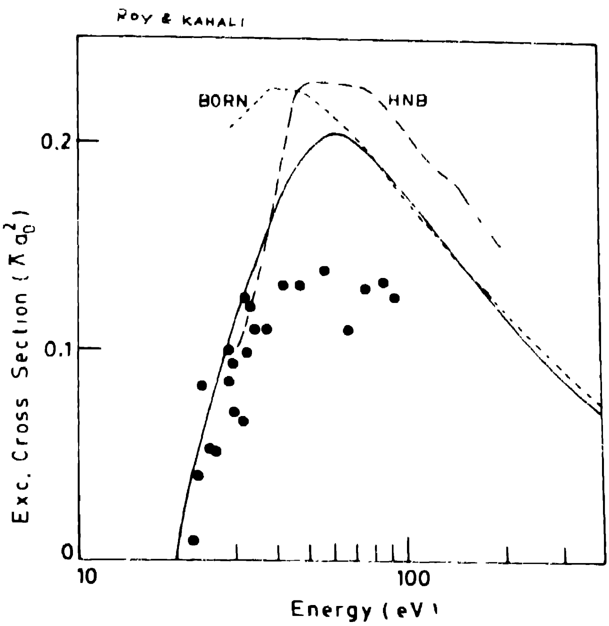

Figure 2. Partial summed total excitation cross sections of He ($1s\,2^1s$) and He ($1s\,2^1P$) states shown in full line. Dotted line is the Born calculation The dashed lines, HNB is CCA calculation of Hewitt *et al* [9] ●, Experimental points (Sueoka as quoted by Charlton and Laricchia [17])

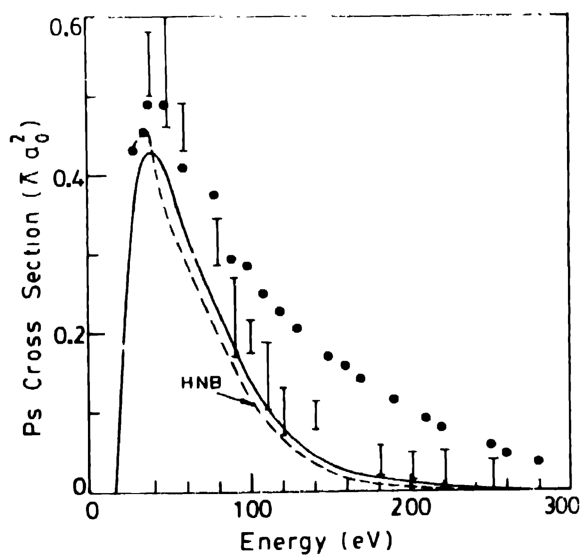

Figure 3. Total Ps-formation cross section, -   -, Present result ; - - - -, HNB (Hewitt *et al* [9]) result. The experimental points denoted by error bars (Overton *et al* [18]) and ● Fromme *et al* [20]).

Total Ps formation cross sections at intermediate energies have been recently measured by Overton *et al* [18]. We define the total Ps formation cross section as

$$\sigma_{Ps} = \sigma_{1s} + \sigma_{2s} + \sigma_{2p}.$$

We have taken $n = 2$ excitation cross section from Khan *et al* [19]. We compare our total Ps formation cross sections with measured data of Overton *et al* [18] and Fromme *et al* [20] in Figure 3. The results of HNB are also plotted in the same figure. The present results are in fair agreement with the measured data of Overton *et al* beyond 80 eV. The predictions of HNB are in good accord with those of 4-state CCA except near the threshold energy.

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