THEORETICAL SURVEY ON POSITRONIUM FORMATION AND IONISATION IN
POSITRON ATOM SCATTERING

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ABSTRACT

The present survey reports the recent theoretical studies on the formation of exotic atoms in positron-hydrogen, positron-helium and positron-lithium scattering specially at intermediate energy region. The ionisations of these targets by positron impact has also been considered. Theoretical predictions for both the processes are compared with existing measured values.

INTRODUCTION

In recent years, amazing developments in the studies of positron-atom scattering have been noticed. It has become possible due to the availability of intense and energy resolved positron beam and sensitive detectors. A large number of parallel theoretical studies, in recent years, also play a big role in it. The present survey concentrates on the recent theoretical developments in the studies of inelastic processes in e⁺-atom scattering. In particular, we discuss on the following two inelastic processes.

i) Positronium formation in e⁺-atom scattering;
ii) Ionisation of atoms by positron impact.

These two inelastic processes are not altogether different. Positronium atom may also be formed in the continuum. This has been first predicted by Brauner and Briggs that the presence of (e⁺-e⁻) pair in the final state of positron impact ionisation results in a process known as 'positronium to the continuum'. This is due to the energy distribution of the secondary electron. The London group (Charlton et al) reported the first experimental evidence for a peak in the energy distribution of the secondary electrons from positron impact ionisation.

In the last conference on Positron in Gases in 1987, the topic has been discussed in details. It is of no use to repeat this.

In the last workshop on Positron in Gases, there are little discussion about the theoretical models employed to investigate these two important inelastic processes, although, results are quo-
ted many times by different speakers. However, theoretical models are covered by Ghosh in our national conference. In this resume, we discuss the theoretical models developed or employed to investigate these two inelastic processes after 1986.

Due to the limited time, we will consider H, He and Li atoms as targets. We start with positronium formation in $e^+\text{-atom}$ scattering.

Positronium Formation

Positronium (Ps), the decaying bound state of the electron and its antiparticle has presented an alluring challenge to experimentalists and theoretical physicists for over 35 years. Milestones in positronium research includes the observation of its ground state in 1951, observation of its excited state in 1975 and recent dramatic discovery of positronium negative ion (Ps$^-$) in 1981. Positronium atom, in its ground and excited states may be formed in $e^+$-atom and $e^+$-molecule collisions. A large number of theoretical studies have been carried out to predict capture cross sections using different theoretical models depending on the energy range considered. For earlier works one may go through a series of excellent reviews (Ghosh et al., Humberston, Ghosh and Joachain).

We start with Ps-formation in $e^+$-He scattering. This is due to the fact that maximum number of experiments have been carried out for this system (Fornari et al., Charlton et al., Fromme et al., Diana et al.). A large number of theoretical investigations have also been made during the same period. Mandal et al. have carried out a distorted wave model to predict ground state capture whereas Khan and Ghosh and Khan et al. have reported ground and excited state capture cross section respectively using distorted wave polarized orbital method. McDowell and Peach have also investigated the same process using classical theory of charge transfer. To have an idea about the agreement between the theoretical predictions and measured values, we compare the Ps formation cross sections ($\sigma_{Ps}$) in Fig.1. It is evident from Fig.1 that all experimental results except those of Charlton et al. are in fair agreement with one another. Here, measured

$$\sigma_{Ps} = \sigma_{Ps}^{(1s)} + \sigma_{Ps}^{(all \ excited \ states)}$$

whereas theoretically

$$\sigma_{Ps} = \sigma_{Ps}^{(1s)} + \sigma_{Ps}^{(2s)} + \sigma_{Ps}^{(2p)}$$

as calculated by Khan et al.

At higher energies, theoretical results seem to underestimate $\sigma_{Ps}$.
Ps formation in an \( e^+ \)-atom collision can be compared with electron transfer in a proton-atom collision. It is well known that in ion-atom scattering, the second Born term is of vital importance in determining the asymptotic behaviour of the capture cross section. Considering these facts, we have used a model in which the second-order effects are included in a realistic way. We have employed two second order models to calculate ground state capture cross sections. These models may be represented by the following two equations:

\[
\begin{align*}
S_{\text{BA}} &= g_{\text{B1}} + g_{\text{B2}} \\
S_{\text{CG}} &= g_{\text{CS}} + g_{\text{B2}}
\end{align*}
\]

where \( g_{\text{B1}} \) is the first Born capture amplitude and \( g_{\text{CS}} \) is the capture amplitude obtained by solving coupled static equations. \( g_{\text{B2}} \) is the conventional second Born term. \( g_{\text{B2}} \) is given by

\[
\tilde{g}_{\nu',\nu}^{\text{B2}}(k',k) = \frac{1}{2\pi^2} \sum_{\nu''=1s} \int \frac{g_{\nu''}}{(k''^2-k_y'^2-i\epsilon)} \times g_{\nu',\nu''}(k'',k) f_{\nu',\nu}(k''',k) \]

where \( g_{\nu',\nu''}(k'',k) \) and \( f_{\nu',\nu}(k'',k) \) are the first Born amplitudes in the direct and rearrangement channel respectively. In other words, in calculating \( \tilde{g}_{\nu',\nu}^{\text{B2}} \), the summation over the ground state is omitted. Closure relation is found to be unsuitable in evaluating the second Born capture amplitude. The second Born terms \( g_{\text{B2}} \) and \( \tilde{g}_{\text{B2}} \) are evaluated by retaining suitably chosen target states.

a) Hydrogen Atom

We have started the investigations with hydrogen atom (Basu and Ghosh) as this is the trial horse for the theoreticians as
most accurate results are available or may be performed only in case of hydrogen atom. To have reliable results, convergence of the second Born term with the addition of the target state is required. We have retained two eigenstates (1s, 2s) and three pseudo-states (2p, 3s and 3d). The pseudo states 2p and 3d are taken from Damburg and Karule\textsuperscript{15} and 3s from Burke and Webb\textsuperscript{16}. To justify our choice of pseudo-states, we have evaluated the direct second Born amplitudes using these states. Table 1 gives the forward second Born amplitude for elastic $e^{-}-H$ scattering along with those of Holt\textsuperscript{17} and Prasad\textsuperscript{18}.

Table 1. Forward second Born amplitude for elastic $e^{-}-H$ scattering (atomic unit).

<table>
<thead>
<tr>
<th>E (eV)</th>
<th>50</th>
<th>100</th>
<th>300</th>
</tr>
</thead>
<tbody>
<tr>
<td>Real</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exact*</td>
<td>1.96</td>
<td>1.35</td>
<td>C.74</td>
</tr>
<tr>
<td>BG</td>
<td>1.75</td>
<td>1.25</td>
<td>0.65</td>
</tr>
<tr>
<td>Imaginary</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exact*</td>
<td>1.60</td>
<td>1.51</td>
<td>1.15</td>
</tr>
<tr>
<td>BG</td>
<td>1.76</td>
<td>1.54</td>
<td>1.14</td>
</tr>
</tbody>
</table>

*Holt 10, Prasad 11.

Present results are in reasonably good agreement with those of exact predictions as given by Holt and Prasad. This is the reason behind our choice of Pseudo-state in the calculation.

We have calculated the differential cross section (DCS) for ground state capture in the energy range 50-300 eV using conventional second Born approximation (SBA) and in the energy range 50-200 eV by using model (2) (denoted by BG). Fig. 2 and 3 show our DCS using BG.

Fig. 2. Differential cross sections (DCS) ($a^2$ sr$^{-1}$) for ground state capture in $e^{-}-H$ scattering at 80 eV; ---, BG; --, SBA; ----, FBA.

Fig. 3. Same as Fig. 2 but at 300 eV and SBA at the energies 80.0 and 300.0 eV. The results of the first Born approximation (FBA) have also been included. The FBA results attain a zero value around the scatter-
ring angle $25^\circ$, whereas the SBA and BG have structures near $45^\circ$. The FBA predicts zero cross section as the two parts of the amplitude are of opposite sign. The second order term prevents the total cancellation in the DCS and the residual structure is due to the destructive interference of the amplitudes. The Thomas peak for electron capture by heavier atoms is well known. For the $p^+ - H$ system, there are two peaks. In case of positron capture, the two peaks approach at about $45^\circ$. These features have been noticed by us at all energies.

Recently, Deb et al.\textsuperscript{19} have applied a second Born approximation in which Green's function is evaluated approximately to investigate the problem. In Fig. 4, we compare our SBA results with those of Deb et al.\textsuperscript{19} (DMS) at the incident energy 1360 eV. Our SBA structure near $45^\circ$ is more prominent than that of DMS. DMS results fall faster than ours after the scattering angle $50^\circ$. There is no reason to prefer one result over other. The results await experimental confirmation or more elaborate calculations.

Integrated cross sections for ground-state capture using SBA and BG are given in Table 2, along with FBA and coupled static results (CSA). The BG and SBA results are always greater than that of the FBA and the present values (BG) lies between those of FBA and SBA except at the lowest energy considered here (50 eV). From the table it is evident that the BG results are always less than the CSA results. It may be mentioned that the DMS results of Deb et al and DWPO results of Khan and Ghosh (not shown in the table) are always less than the present SBA and FBA results respectively.

We have extended our SBA to calculate n=2 excited state cap-

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>FBA</th>
<th>CSA</th>
<th>SBA</th>
<th>BG</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>0.46</td>
<td>0.55</td>
<td>0.62</td>
<td>0.56</td>
</tr>
<tr>
<td>80</td>
<td>0.10</td>
<td>0.13</td>
<td>0.13</td>
<td>0.12</td>
</tr>
<tr>
<td>100</td>
<td>0.46$^{-1}$</td>
<td>0.51$^{-1}$</td>
<td>0.53$^{-1}$</td>
<td>0.46$^{-1}$</td>
</tr>
<tr>
<td>200</td>
<td>0.25$^{-2}$</td>
<td>0.28$^{-2}$</td>
<td>0.31$^{-2}$</td>
<td>0.26$^{-1}$</td>
</tr>
<tr>
<td>300</td>
<td>0.37$^{-3}$</td>
<td>0.40$^{-3}$</td>
<td>0.49$^{-3}$</td>
<td>0.39$^{-3}$</td>
</tr>
<tr>
<td>500</td>
<td>0.26$^{-4}$</td>
<td>-</td>
<td>0.38$^{-4}$</td>
<td>-</td>
</tr>
</tbody>
</table>
ture in $e^+\text{-H}$ scattering. Second Born term is evaluated by retaining three eigenstates ($1s, 2s, 2p$) of the target atom. Tripathi, Sinha and Sil have also predicted excited state ($n=2$) capture cross section using eikonal approximation. Fig. 5 shows the DCS for 2s state capture at the incident energies 80.0 and 500.0 eV. The FBA, as usual, predicts the zero cross section at all the energies. No structure is obtained in the DCS using the SBA upto the incident energy 100 eV. As the energy increases, the structure is more prominent and the position of the structure is around 45°. We show only the results at 500.0 eV. The contribution of the second order terms is dominant around the zero values of the FBA at low energies. At high energies, these terms prevent total cancellation and we get the residual structure. However Khan et al using their distorted wave method have obtained structure for the same processes even at 13.6 eV.

Our DCS for the 2p-state capture process at 80 and 500 eV are shown in Fig. 6. As in the case of
amplitudes are combined. The second Born term is totally responsible for the structure at high energies. In fact, the destructive interference of the FBA and the SBA amplitudes at high energies provides the structure. We hasten to add that Thomas mechanism is valid only at high energies. Therefore, it is not surprising that we have not obtained Thomas peak for excited state capture at low energies.

Table 3 presents the integrated excited state capture cross sections.

Table 3. Integrated SBA cross section ($\pi a_0^2$) for excited (2s and 2p) state capture in $e^+\cdot H$ scattering.

<table>
<thead>
<tr>
<th>E (eV)</th>
<th>2s</th>
<th>2p</th>
</tr>
</thead>
<tbody>
<tr>
<td>50.0</td>
<td>0.165</td>
<td>0.366^-1</td>
</tr>
<tr>
<td>80.0</td>
<td>0.252^-1</td>
<td>0.601^-2</td>
</tr>
<tr>
<td>100.0</td>
<td>0.124^-1</td>
<td>0.239^-2</td>
</tr>
<tr>
<td>200.0</td>
<td>0.507^-3</td>
<td>0.620^-4</td>
</tr>
<tr>
<td>300.0</td>
<td>0.699^-4</td>
<td>0.663^-5</td>
</tr>
<tr>
<td>500.0</td>
<td>0.534^-5</td>
<td>0.348^-6</td>
</tr>
</tbody>
</table>

The present second Born results are always greater than those of the FBA. These results are of importance to obtain the total Ps-formation cross section. The present excited state capture cross section are not negligible when compared with ground state capture cross sections. It may be noted that 2s and 2p state capture cross sections differ by one order of magnitude, 2s state capture cross section being higher.

To find the validity of our methods, our group has carried out investigations using close coupling approximation (CCA) with two coupling schemes

1) $H(1s), H(2s), H(2p), Ps(1s)$
2) $H(1s), H(2s), H(2p), Ps(1s)$

Instead of solving the conventional coupled integro-differential equations, we recast the Schrodinger equation into a coupled integral equation in the momentum space. The final one-dimensional coupled integral equations have been solved by matrix inversion method. The details of the numerical method have been discussed in our paper (Basu, Mukherjee and Ghosh21).

At low incident energies (in the core-gap region) very reliable s-, p- and d-wave ground state capture cross sections for $e^+\cdot H$ are available (Humberston and his co-workers22-24) using variational methods. In practice, it is not possible to perform such elaborate calculation at intermediate and high energies and also for complex systems. We compare two sets of s, p and d-wave phase shifts obtained using CCA with variational results in Tables 4 - 6.

It is well known that the s-wave Ps-formation cross section is very sensitive to the method employed. In Table 1, we have shown pre-
sent two sets of results along with

Table 4. s-wave positronium formation cross sections (\(\pi a_0^2\)).

<table>
<thead>
<tr>
<th>k</th>
<th>1s-2s-2p-Ps</th>
<th>1s-2s-2p-Ps</th>
<th>H(^22)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.71</td>
<td>608(-2)</td>
<td>558(-3)</td>
<td>41(-2)</td>
</tr>
<tr>
<td>0.75</td>
<td>418(-2)</td>
<td>282(-3)</td>
<td>44(-2)</td>
</tr>
<tr>
<td>0.8</td>
<td>244(-2)</td>
<td>113(-2)</td>
<td>49(-2)</td>
</tr>
<tr>
<td>0.85</td>
<td>156(-2)</td>
<td>-</td>
<td>58(-2)</td>
</tr>
</tbody>
</table>

the variational prediction (Humberston\(^22\)).

Table 5. p-wave positronium formation cross section (\(\pi a_0^2\)).

<table>
<thead>
<tr>
<th>k</th>
<th>1s-2s-2p-Ps</th>
<th>1s-2s-2p-Ps</th>
<th>BH(^23)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.71</td>
<td>121(-1)</td>
<td>803(-2)</td>
<td>27(-1)</td>
</tr>
<tr>
<td>0.75</td>
<td>278</td>
<td>218</td>
<td>37</td>
</tr>
<tr>
<td>0.8</td>
<td>411</td>
<td>344</td>
<td>48</td>
</tr>
<tr>
<td>0.85</td>
<td>470</td>
<td>401</td>
<td>56</td>
</tr>
</tbody>
</table>

In Tables 5 and 6 we have tabulated our present two sets of p- and d-wave capture cross sections. The

Table 6. d-wave positronium formation cross section (\(\pi a_0^2\)).

<table>
<thead>
<tr>
<th>k</th>
<th>1s-2s-2p-Ps</th>
<th>1s-2s-2p-Ps</th>
<th>BH(^24)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.71</td>
<td>286(-3)</td>
<td>351(-3)</td>
<td>62(-3)</td>
</tr>
<tr>
<td>0.75</td>
<td>144</td>
<td>170</td>
<td>34</td>
</tr>
<tr>
<td>0.78</td>
<td>465</td>
<td>578</td>
<td>81</td>
</tr>
<tr>
<td>0.85</td>
<td>684</td>
<td>897</td>
<td>11(+1)</td>
</tr>
</tbody>
</table>

variational results (Brown and Humberston\(^23\)) have also been included for comparison. Our p- and d-wave cross sections are in fair agreement with variational numbers the present numbers being lower.

The polarizability of Ps atom is eight times that of hydrogen. It is expected that the inclusion of long range force of the Ps atom will affect the results significantly.

Being encouraged by the above results, we have carried out our CCA calculations up to the incident energy (200 eV) (Mukherjee et al\(^25\)).

Fig. 7 shows the present differential cross section at 100 eV using our second order results (BG) along with our two models of CCA at 100 eV. The position of the Thomas peak as obtained using eigen state CCA and BG are nearly identical whereas pseudo-state CCA fails to predict the Thomas peak. However, we may skip the minimum. At large scattering angles, the two sets of CCA results differ appreciably from BG. The contribution to the scattering amplitude up to the second order may not be sufficient for.
convergent results at large scattering amplitude up to the second order may not be sufficient for convergent results at large scattering angles. This may be the reason of discrepancy.

Table 7 presents the ground state capture cross sections obtained by different methods. BG and SBA are the two second order results. Our pseudo-state CCA and the FBA results are also included for comparison. For incident energies \( E = 100 \text{ eV} \), our CCA and BG results are in good agreement. It is interesting to note, even at 300 \text{ eV}, the second order results BG and SBA are greater than the FBA results.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
\textbf{E (eV)} & 50 & 100 & 200 & 300 \\
\hline
\textbf{Pseudo} & 0.37 & 0.46 \(^{-1}\) & 0.27 \(^{-2}\) & - \\
\textbf{SBA} & 0.62 & 0.53 \(^{-1}\) & 0.31 \(^{-2}\) & 0.49 \(^{-3}\) \\
\textbf{BG} & 0.56 & 0.46 \(^{-1}\) & 0.26 \(^{-2}\) & 0.39 \(^{-3}\) \\
\textbf{FBA} & 0.46 & 0.46 \(^{-1}\) & 0.25 \(^{-2}\) & 0.37 \(^{-3}\) \\
\hline
\end{tabular}
\caption{Ground state capture cross section (in units of \( \pi a_0^2 \)).}
\end{table}

*54.4 eV results.

b) Helium Atom

Deb et al.\(^{26}\) have calculated ground state capture cross section using similar method as applied to the case of hydrogen atom in the high energy region. Here also, they have obtained the structure in the DCS around 50\(^{0}\) as expected. Their ground state capture cross sections in the very high energies are also greater than the corresponding BK results. We are now investigating the same process using our FBA to calculate \( \sigma^{PS} \). Till now, we are able to include three eigenstates (1s\(^2\), 2\(^1\)s, 2\(^1\)p) as intermediate one. Our preliminary result shows that cross section is increased by about 10\(^{\circ\text{C}}\) over FBA at the incident energy 300 \text{ eV}. Below this incident energy, results may not be be reliable. Fig. 8 shows the diffe

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig8.png}
\caption{DCS in \( \text{e}^+\text{-He} \) ground state capture (\( a_0^2 \text{sr}^{-1} \)). --, SBA, ---, FBA.}
\end{figure}

rential cross section at 300.0 \text{ eV} using FBA and SBA for ground state capture in \( \text{e}^+\text{-He} \) scattering.

c) Lithium Atom

Recently, Abdel-Rauf\(^{27}\) has employed a frozen-core coupled static method to investigate \( \text{e}^+\text{-Li} \)
and $e^+-$Na scattering. The effect of the inner shell is taken by introducing a core potential. Moreover, the exchange effect of the valence electron with those of core is included via local exchange potential. He has reported the results up to the incident energy 1000.0 eV. Using the wavefunction of Clementi and Ropetti.

In the present conference, Ghosh and Basu also report the coupled static calculations using the wavefunction of Weiss. In our calculation, we assume that the valence electron is the only active electron. As the valence electron lies well outside the core, this we expect, introduces marginal error. At low incident energies (5 eV) results differ appreciably from those of Abdel-Rauf (Table 8). We believe.

Table 8. Total ground state capture cross section ($\sigma_{\text{ion}}$) using coupled static approximation.

<table>
<thead>
<tr>
<th>E(eV)</th>
<th>Ghosh et al.</th>
<th>Abdel Raouf</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>137.8</td>
<td>140.9</td>
</tr>
<tr>
<td>0.5</td>
<td>87.2</td>
<td>47.3</td>
</tr>
<tr>
<td>1.0</td>
<td>51.94</td>
<td>51.43</td>
</tr>
<tr>
<td>3.0</td>
<td>35.35</td>
<td>16.9</td>
</tr>
<tr>
<td>5.0</td>
<td>24.5</td>
<td>14.3</td>
</tr>
</tbody>
</table>

The difference between these two results are due to the use of different wavefunctions as well as with and without inclusion of exchange core potential. We also report our preliminary results using 2s, 2p, ps CCA in this conference. It may be mentioned that we have also calculated the ground and $n=2$ state capture cross sections for $e^+-$Li scattering (Sarkar et al. 31, 32) using the second order method of Basu and Ghosh at intermediate energies.

ii) Ionisation

a) Helium Atom

We concentrate mainly on total ionisation cross section ($\sigma_{\text{ion}}$) in $e^+-$He scattering as three groups (Fromme et al 8, Diana et al 9, Sueoka 33) have measured $\sigma_{\text{ion}}$ for this system in this decade. The first quantum mechanical calculation for $e^+-$He ionisation including the positron signature has been carried out by us (Basu et al 34). The choice of the effective charges are as follows:

\[ Z_A \quad Z_B \]

i) 1 1

ii) 0 1

A distorted wave method in which the wavefunction of the incoming positron $F(X)$ satisfies the adiabatic Schrödinger equation given by

\[ (\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_S(x) + V_P(x)) F(x) = 0 \]

has been employed to investigate the problem. Here $V_S$ and $V_P$ are the static and polarization potentials respectively. The Hylleraas wavefunction has been used for computational
ease. The distortion in the initial channel is found to be insignificant. Campeanu et al.\textsuperscript{35} have repeated the calculation using Hartree-Fock wavefunction from Clementi and Roetti for $e^+\cdot$He ionisation with certain modifications and using different distorted wave models. They have considered following different choices of effective charges

\[
\begin{array}{ccc}
Z_A & Z_B \\
i) & 1 & 1 \\
i) & 0 & 0 \\
iii) & 0 & 1 \\
v) & 0 & 1 \\
\end{array}
\]

They argued that model (ii) of Basu et al.\textsuperscript{34} is not physically correct because when the ejected electron is faster than the scattered positron, it cannot screen the residual ion. In other words, they have taken the maximum value of the energy of the ejected electron to be $E/2$. Moreover, they have taken the distortion in the final channel.

In Fig. 9, the theoretical predictions for total ionisation cross section ($\sigma_{\text{ion}}^+$) in $e^+\cdot$He scattering are compared with the measured values of Fromme et al.\textsuperscript{33}. The agreement between the theoretical results and measured values is good.

b) Hydrogen Atom

Very recently, Spicher et al.\textsuperscript{36} have measured $\sigma_{\text{ion}}$ for $e^+\cdot$H scattering. It may be mentioned that we (Ghosh et al.\textsuperscript{37}) have performed the calculations for $e^+\cdot$H ionisation using the same method.
as applied $e^+\text{-He}$ ionisation. Recently Mukherjee et al. have also investigated $e^-\text{-H}$ ionisation following Campeanu et al. Theoretical results are compared with measured values in Fig.10. It is found that results of Ghosh et al are in good agreement with the measured values. Results of Mukherjee et al are in good agreement with the measured values. Results of Mukherjee et al are lower than those of Ghosh et al and are in fair agreement with the experimental values.

(c) Lithium atom

Basu and Ghosh have calculated $\sigma_{\text{ion}}$ in $e^+\text{-Li}$ collision using distorted wave method. The ionisation cross section is found to be very small when compared to elastic or other inelastic processes. In absence of any elaborate work or experimental measurements, there is no scope for comparison.

However, we like to point out certain salient features of ionisation process.

Theory of ionisation of atoms by electron and positron impact is complicated due to the role of Coulomb correlation in the asymptotic behaviour of ionised electron. Peterkop-Rudge-Seaton theory of ionisation offers the prescription for the final state wavefunction and their relation between the effective charges $Z_A$ and $Z_B$ in the final state wavefunction is given by

$$\frac{Z_A}{k_A} + \frac{Z_B}{k_B} = \frac{1}{k_B} - \frac{1}{|k_A - k_B|}$$

In the literature, we have found different choices for the effective charges satisfying the above relation but otherwise arbitrary. It is not possible to find an unique relation between the charges. The ionisation cross section is extra-sensitive to the choice of the final state wavefunction (Ghosh et al). This is apparent from Fig.11. Here

Fig.11. Triple differential cross section (TDCS) at $e^+\text{-H}$ ionisation at $E = 20$ eV ($E_2 = 3$ eV, $\theta_1 = 20^\circ$): $\cdots\cdots$, FBA; $\cdots\cdots$, choice (ii) of Ghosh et al; $\cdots\cdots$, DCA (multiplied by a factor of $10^3$).

The results of triple differential cross section (TDCS) using double Coulomb approximation (DCA) differ from those of the Born results by a factor of $1000$. The results using the other choices are also found to differ dramatically.

To study the ionisation process, one, we believe, has to be very careful regarding the asymptotic condition prescribed by Peterkop-
Moreover, the effective charges should fulfill the following limiting conditions which must be satisfied physically.

i) \( k_A \to \infty \) or \( k_B \to 0 \) and \( k_A > k_B \), the effective charges must behave as \( Z_A \to 0 \) and \( Z_B \to 1 \).

ii) In the symmetric case i.e. \( |k_A| = |k_B| \), the effective charges must be equal i.e. \( Z_A = Z_B \).

Recently, Faisal and his co-workers have initiated studies to investigate ionisation processes in this light. They tried to get the values of the effective charges by exploiting Peterkop-Rudge-Seaton prescription and above two limiting conditions. Amongst their six unknown parameters, they have been able to solve five in terms of one. They tuned the unknown parameter with the triple differential cross section at one incident energy and at one angle. This is a limitation in their approach which of course authors are aware of. Moreover, this is not an unique way to solve the problem. We advocate one should study the ionisation process removing the arbitrary character in the choice of effective charges as far as practicable.

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