Proton scattering from excited states of atomic hydrogen + some other processes

A S Kadyrov
and
I B Abdurakhmanov, Sh U Alladustov, J J Bailey, I Bray

Curtin University, Australia

2nd RCM, IAEA, Vienna 2019
Outline

① Single-centre semiclassical close-coupling (CC) approach
② Difficulties associated with two-centre semiclassical CC approach
③ Two-centre semiclassical convergent close-coupling (CCC) approach
④ Total and various differential cross sections for ionisation and electron capture in following collisions
  ▪  \( p + H(n=2) \)
  ▪  \( C^6+ + H(1s) \)
  ▪  \( p + He(1s^2) \)
  ▪  \( H(1s) + H(1s) \)
1-centre semiclassical CC approach

A lab frame: the origin at the target, \( z \)-axis \( \parallel \) \( \vec{v} \) and \( x \)-axis \( \parallel \) \( \vec{b} \)

Projectile position
\[
\vec{R}(t) = \vec{b} + \vec{Z} = \vec{b} + \vec{v}t
\]

The w.f. is a solution to SC TDSE
\[
i \frac{\partial \Psi(\vec{r},t)}{\partial t} = (H_T + V_p) \Psi(\vec{r},t)
\]

Expand \( \Psi \) in terms of pseudostates of \( H_T \)
\[
\Psi(\vec{r},t) = \sum_\alpha a_\alpha(t) \exp(-i\varepsilon_\alpha t) \phi_\alpha(\vec{r})
\]
1-centre semiclassical approach

Then we get

\[ i \dot{a}_\alpha(t) = \sum_\beta \exp[i(\varepsilon_\alpha - \varepsilon_\beta)t]a_\beta(t)D_{\alpha\beta} \]

\[ D_{\alpha\beta} = \langle \phi_\alpha \mid -\frac{1}{R(t)} + \sum_i \frac{1}{|\vec{r}(t) - \vec{r}_i|} \mid \phi_\beta \rangle \]

In matrix form

\[ i \dot{a} = Da \]

Pseudostates

\[ \langle \phi_\beta \mid H_T \mid \phi_\alpha \rangle = \delta_{\beta\alpha}\varepsilon_\alpha \]
Conventional 2-centre CC approach

In 1-centre case we used

$$\Psi(\vec{r}_A, t) = \sum_\alpha a_\alpha(t) \phi_\alpha^A(\vec{r}_A) e^{-i\varepsilon_\alpha t}$$

It is a solution to TDSE

$$i \frac{\partial \Psi(\vec{r}_A, t)}{\partial t} = (H_A + V_B) \Psi(\vec{r}_A, t)$$

• Now we take into account electron capture
• We need a 2-centre expansion
Conventional 2-centre CC approach

2-centre expansion

\[ \Psi(\vec{r},t) = \sum_{\alpha} a_{\alpha}(t) \phi_{\alpha}^{A}(\vec{r}_A) e^{-i\varepsilon_{\alpha}t} + \sum_{\beta} b_{\beta}(t) \phi_{\beta}^{B}(\vec{r}_B) e^{-i\varepsilon_{\beta}t} \]

There are 2 problems
We write TDSE in c.m. frame

\[ i \frac{\partial \Psi(\vec{r},t)}{\partial t} = (T_{\vec{r}} + V) \Psi(\vec{r},t) \]

However, this does not solve the problem.
The wave function does not satisfy boundary conditions.
Electronic translational factors

Bates and McCarroll (1958): electronic translational factors (ETF)

2-centre expansion satisfying the boundary conditions

\[\Psi(\vec{r},t) = \sum_{\alpha} a_{\alpha}(t)\phi_{\alpha}^{A}(\vec{r}_{A})e^{-i\epsilon_{\alpha}t+i\pi_{\alpha}^{A}(\vec{r},t)-iv^{2}t/8} + \sum_{\beta} b_{\beta}(t)\phi_{\beta}^{B}(\vec{r}_{B})e^{-i\epsilon_{\beta}t+i\pi_{\beta}^{B}(\vec{r},t)-iv^{2}t/8}\]

where \(\pi_{\alpha}^{A}(\vec{r},t)\) and \(\pi_{\beta}^{B}(\vec{r},t)\) are arbitrary functions.

The only condition is that when \(|t| \rightarrow \infty\)

\[\pi_{\alpha}^{A}(\vec{r},t) \rightarrow -\frac{1}{2} \vec{v}\vec{r} \quad \text{and} \quad \pi_{\beta}^{B}(\vec{r},t) \rightarrow \frac{1}{2} \vec{v}\vec{r}\]
Science of ETFs

- There is a non-uniqueness problem

- Choice of ETFs and their optimisation (using variational techniques) become elaborate science

- Types of ETFs:
  - common
  - state-dependent
  - plane-wave
  - non-PW etc

- Many papers and reviews have been published
- Bates and McCarroll (1958) solution was incomplete
- We believe there is a better solution
2 problems with the standard approach

- Bates and McCarroll (1958) solution was incomplete
- There is no need for an ad-hoc solution using as ETF
- The reason for the problem was 2-fold

1st problem appears in the attempt to represent the 2nd centre w.f. in the same form as the w.f. of the 1st centre

\[
\Psi(\vec{r}, t) = \sum_\alpha a_\alpha(t) \phi_\alpha^A(\vec{r}_A) e^{-i\epsilon_\alpha t + i\pi_\alpha^A(\vec{r}_A) - iv^2 t/8} + \sum_\beta b_\beta(t) \phi_\beta^B(\vec{r}_B) e^{-i\epsilon_\beta t + i\pi_\beta^B(\vec{r}_B) - iv^2 t/8}
\]

2nd problem is in TDSE
What is the solution?

- The correct 1-centre expansion should look like

\[ \Psi(\vec{r}, t) = \sum_{\alpha} a_\alpha(t) \phi^A_\alpha(\vec{r}_A) e^{-i\epsilon_\alpha t} \Rightarrow \tilde{\Psi}(\vec{r}, t) = \sum_{\alpha} a_\alpha(t) \phi^A_\alpha(\vec{r}_A) e^{i\kappa_\alpha \sigma} \]

- Both satisfy the semi-classical TDSE

\[ i \frac{\partial \Psi(\vec{r}, \vec{b}, t)}{\partial t} = (T_r + V) \Psi(\vec{r}, \vec{b}, t) \]

- But \( \tilde{\Psi} \) also satisfies the full (exact) TISE

\[ (E - H) \tilde{\Psi} = 0 \]
How does temporal factor emerge?

\[(k_{\alpha} - k_{\alpha'}) \cdot \sigma \approx (k_{\alpha} - k_{\alpha'}) \cdot R = q_{\parallel} z + q_{\perp} \cdot b\]

\[q_{\parallel} = (\epsilon_{\alpha'} - \epsilon_{\alpha}) / \nu\]

Since \(z = \nu t\)

\[(k_{\alpha} - k_{\alpha'}) \cdot \sigma \approx (\epsilon_{\alpha'} - \epsilon_{\alpha}) t + q_{\perp} \cdot b\]
What is the solution?

- The correct 2-centre expansion is

\[
\tilde{\Psi}(\vec{r}, t) = \sum_{\alpha} a_\alpha(t) \phi_\alpha^A(\vec{r}_A) e^{i\vec{k}_\alpha \vec{\sigma}} + \sum_{\beta} b_\beta(t) \phi_\beta^B(\vec{r}_B) e^{i\vec{k}_\beta \vec{\rho}}
\]

- This w.f. does not satisfy TDSE

\[
i \frac{\partial \tilde{\Psi}(\vec{r}, t)}{\partial t} \neq (T_{\vec{r}} + V) \tilde{\Psi}(\vec{r}, t)
\]

- But satisfies the full TISE \((E - H) \tilde{\Psi} = 0\)
How does ETF appear?

\[ k_\beta \cdot \sigma_P - k_{\alpha'} \cdot \sigma_T = p_{\beta \parallel} z + p_{\beta \perp} \cdot b + v \cdot r_T \]

\[ p_{\beta \parallel} = -\frac{v}{2} + \frac{(\epsilon_{\alpha'} - \epsilon_\beta)}{v} \]

\[ k_\beta \cdot \sigma_P - k_{\alpha'} \cdot \sigma_T = (\epsilon_{\alpha'} - \epsilon_\beta) t - \frac{v^2 t}{2} + p_{\beta \perp} \cdot b + v \cdot r_T \]

- These 2 terms were introduced *ad-hoc* to fix the problem
- In our approach they appear naturally
- Details: Abdurakhmanov etal, PRA 97, 032707 (2018)
2-centre semi-classical equations

- Inserting $\tilde{\Psi}$ into TISE $(E - H)\tilde{\Psi} = 0$ and using semi-classical approximation we get the same result as we would get using PW ETFs

$$i \begin{pmatrix} I & G^A \\ G^B & I \end{pmatrix} \begin{pmatrix} \dot{a} \\ \dot{b} \end{pmatrix} = \begin{pmatrix} D^A & Q^A \\ Q^B & D^B \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$$

NB: Compare with 1-centre case: $i\dot{a} = D^A a$

- Thus there is no SC TDSE when rearrangement included
Wave-packet continuum discretisation

\[\phi_{il}^{WP}(r) = \frac{1}{\sqrt{w_i}} \int_{k_{i-1}}^{k_i} dk \phi_{kl}(r)\]

Coulomb function

\[\langle \phi_{jl}^{WP} | H_T | \phi_{il}^{WP} \rangle = \delta_{ji} \varepsilon_i\]

Box Advantages of WP: there are 3

\[\langle \psi_k | \phi_f \rangle = \sqrt{\frac{2}{\pi}} (-i)^l e^{i\sigma_i} b_{nl}(k) Y_{lm}(\hat{k})\]

\[b_{nl}(k) = \int_0^{\infty} dr \varphi_{kl}(r) \varphi_n^{WP}(r) = \frac{1}{\sqrt{w_n}}\]
Ionisation amplitude

\[ T^{\text{post}} = \langle \Phi_0^- | \hat{H} - E | \Psi_i^+ \rangle \]

Surface-integral formulation of scattering theory
Kadyrov et al., Ann Phys 324 (2009) 1516:

\[ T^{\text{post}} \approx \langle \Phi_0^- | l_N (\hat{H} - E) l_N | \Psi_i^+ \rangle \]

\[ = \langle \tilde{q}_f, \psi_{\tilde{k}}^- | l_N (\hat{H} - E) l_N | \Psi_i^{N^+} \rangle = \sum_{n=1}^{N} \langle \psi_{\tilde{k}}^- | \phi_n \rangle \langle \phi_n, \tilde{q}_f | \hat{H} - E | \Psi_i^{N^+} \rangle \]

\[ = \langle \psi_{\tilde{k}}^- | \phi_f \rangle \tilde{T}_{fi} \quad \text{for} \quad k^2 / 2 = \epsilon_f \]
Breakup amplitude including ECC

Surface-integral formulation of scattering theory:

\[ T^{\text{post}} = \left\langle \Phi_0^- | \mathcal{H} - E | \Psi_i^+ \right\rangle \approx \left\langle \Phi_0^- (l_N^T + l_M^P) | \mathcal{H} - E | (l_N^T + l_M^P) \Psi_i^+ \right\rangle \]

\[ \equiv \left\langle \Phi_0^- l_N^T | \mathcal{H} - E | \Psi_i^{N|M+} \right\rangle + \left\langle \Phi_0^- l_M^P | \mathcal{H} - E | \Psi_i^{N|M+} \right\rangle \]

Thus the breakup amplitude splits into two:

direct ionisation (DI) and electron capture to continuum (ECC)

\[ T^T = \left\langle \tilde{q}_f, \psi_k^T | l_N (\tilde{H} - E) | \Psi_i^{N|M+} \right\rangle = \left\langle \psi_k^T | \phi_f^T \right\rangle \tilde{T}_{fi}^T \quad \text{for} \quad k^2 / 2 = \varepsilon_f \]

\[ T^P = \left\langle \tilde{q}_f, \psi_p^P | l_P (\tilde{H} - E) | \Psi_i^{N|M+} \right\rangle = \left\langle \psi_p^P | \phi_f^P \right\rangle \tilde{T}_{fi}^T \quad \text{for} \quad p^2 / 2 = \varepsilon_f \]

where \( \psi_k^T \) and \( \psi_p^P \) are the continuum states of target and projectile.
\( p + \text{H}(n=2) \)

**Figure 1.** The weighted elastic \( bP_{2s}^{\text{el}} \), total ionization \( bP_{2s}^{\text{ion}} \) and total electron-capture \( bP_{2s}^{\text{ec}} \) probabilities as a function of impact parameter for 10 keV protons scattering off atomic hydrogen in the 2s state.
Figure 2. Convergence of the elastic, total ionization and total electron-capture cross sections for proton scattering off atomic hydrogen in the metastable 2s state.
Figure 3. The cross sections for super-elastic, elastic and quasi-elastic scattering in p–H(2s) collisions.
Figure 4. The cross sections for excitation of the $n = 3$-shell states in p–H(2s) collisions. The cross sections for excitations to the $p$ and $d$ states are summed over the magnetic quantum number. The CTMC and AOCC-PS results of Pindzola et al [9], and the FBA cross sections are also shown for comparison.
Figure 5. Select electron-capture cross sections for $p$-H(2s) collisions. The CTMC and AOCC-PS calculations of Pindzola et al. [9] (see text) are also shown for comparison. The cross sections for electron-capture to the $p$ and $d$ states are summed over the magnetic quantum number.
Figure 6. Convergence of the elastic, total ionization and total electron-capture cross sections for proton scattering off atomic hydrogen in the $2p_0$ and $2p_1$ states.
Figure 7. The super-elastic, elastic and quasi-elastic scattering, and electron-capture cross sections for proton scattering on atomic hydrogen in the $2p_0$ and $2p_1$ states.
Density matrix

\[ \rho_{\alpha'\alpha}^i = 2\pi \int_0^\infty \, dbbF_{\alpha'\alpha}^*(+\infty, b)F_{\alpha\alpha}(+\infty, b) \]

Table 3. Density matrix elements \( \rho_{\alpha'\alpha}^{2p} \) (in \( 10^{-16} \, \text{cm}^2 \)) for excitation of H(2p1) into the final \( n = 1-4 \) shell states of the target by proton impact at 50 keV.

<table>
<thead>
<tr>
<th>( \alpha' )</th>
<th>( \alpha )</th>
<th>Re</th>
<th>Im</th>
<th>( \alpha' )</th>
<th>( \alpha )</th>
<th>Re</th>
<th>Im</th>
<th>( \alpha' )</th>
<th>( \alpha )</th>
<th>Re</th>
<th>Im</th>
<th>( \alpha' )</th>
<th>( \alpha )</th>
<th>Re</th>
<th>Im</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>200</td>
<td>-1.23</td>
<td>2.32[-1]</td>
<td>210</td>
<td>322</td>
<td>-1.17</td>
<td>-1.28</td>
<td>310</td>
<td>421</td>
<td>2.58[-2]</td>
<td>-2.82[-1]</td>
<td>400</td>
<td>432</td>
<td>-2.96[-2]</td>
<td>2.05[-2]</td>
</tr>
<tr>
<td>100</td>
<td>410</td>
<td>1.35[-2]</td>
<td>1.03[-2]</td>
<td>211</td>
<td>211</td>
<td>13.0</td>
<td>0</td>
<td>311</td>
<td>421</td>
<td>-8.49[-1]</td>
<td>5.82[-1]</td>
<td>410</td>
<td>433</td>
<td>-3.16[-2]</td>
<td>-5.67[-2]</td>
</tr>
<tr>
<td>100</td>
<td>411</td>
<td>-1.93[-1]</td>
<td>2.27[-1]</td>
<td>211</td>
<td>311</td>
<td>-3.90</td>
<td>-6.00[-1]</td>
<td>311</td>
<td>422</td>
<td>-9.26[-1]</td>
<td>-1.17</td>
<td>411</td>
<td>411</td>
<td>4.58[-1]</td>
<td>0</td>
</tr>
<tr>
<td>100</td>
<td>430</td>
<td>8.67[-4]</td>
<td>-1.58[-2]</td>
<td>211</td>
<td>421</td>
<td>1.36</td>
<td>-3.70[-1]</td>
<td>320</td>
<td>320</td>
<td>1.45</td>
<td>0</td>
<td>411</td>
<td>432</td>
<td>1.85[-1]</td>
<td>7.88[-2]</td>
</tr>
</tbody>
</table>

C$_{6}^{+}$ + H(1s) ionisation: test
e-capture and ionisation: convergence

**electron capture**

**ionisation**

![Graphs showing the convergence of electron capture and ionisation cross sections with increasing projectile energy.](image-url)
Electron capture and ionisation
\( ^6\text{C}^+-\text{H} \) DDCS at 1 MeV/amu

C$^{6+}$-H DDCS at 1 MeV/amu

C⁶⁺-H DDCS at 2.5 MeV/amu

C$^{6+}$-H DDCS at 2.5 MeV/amu

Conclusions

- Developed 2-centre CCC approach to HCI-atom collisions including ECC.
- Accurate calculations of the total and various differential cross sections for ionisation and electron capture in p + H and C^6+ + H collisions.
- p + He and H + H collisions.
- C^6+ + H: DDCS and SDCS: good agreement at 2.5 MeV/amu.
- DDCS: some disagreement when low-energy electrons are ejected near the forward direction at 1 MeV/amu.
- SDCS: some disagreement with the experiment seen in the forward direction at 1 MeV/amu.
- p + He: integrated cross sections in good agreement with experiment.
- H + H: good agreement with experiment for electron-loss cross section.
Acknowledgements

Co-authors:

Dr Ilkhom Abdurakhmanov
Dr Jackson Bailey
PhD candidate Shukhrat Alladustov
Prof Igor Bray

This work is supported by Australian Research Council

Thank you for attention!