Convergent Close-Coupling approach to atomic and molecular collisions

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The primary motivation is to provide accurate atomic and molecular collision data for science and industry.

**Collisions on the atomic scale** are difficult to calculate:
- Governed by the Laws of Quantum Mechanics
- Charged particles interact at infinite distances
- Countably infinite discrete spectrum
- Uncountably infinite target continuum
- Can be multicentred (e.g. charge exchange)

Solved by the Convergent Close-Coupling (CCC) method.
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- Astrophysics
  - Fusion research
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- electron-hydrogen excitation or ionisation,
- electron-helium excitation or ionisation,
- single or double photoionisation of helium.

The convergent close-coupling (CCC) theory for electron/positron/photon/(anti)proton collisions with atoms/ions/molecules
- based on a complete $L^2$ expansion of the total wavefunction in the Schrödinger or Dirac equation
- applicable at all energies for elastic, excitation, ionisation and charge exchange processes
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Curtin University
Prior to 2008, no satisfactory mathematical formulation in the case of long-range (Coulomb) potentials for positive-energy scattering in
- Two-body problems
- Three-body problems

Developed a surface integral approach to scattering theory that is valid for short- and long-range potentials
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Extended the CCC method to
- fully relativistic formalism
- multi-centre problems such as positron or proton scattering
- heavy projectiles such as (anti)protons and bare nuclei
- molecular targets: H\textsubscript{2} and H\textsubscript{2}\textsuperscript{+} thus far. Working on Ne-like treatment of H\textsubscript{2}O.
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Using the complete Laguerre basis $\xi_{nl}^{(\lambda)}(r)$ write:

- **“one-electron”** (H, Ps, He$^+$, Li, Na, H$_2^+$, . . .) states: 
  $$\phi_{nl}^{(\lambda)}(r) = \sum_{n'} C_{nl}^{n'} \xi_{n'l}^{(\lambda)}(r)$$

- **“two-electron”** (He, N$^5+$, Be, Hg, H$_2$, . . .) states: 
  $$\phi_{nls}^{(\lambda)}(r_1, r_2) = \sum_{n', n''} C_{nls}^{n'n''} \xi_{n'l'}^{(\lambda)}(r_1) \xi_{n''l''}^{(\lambda)}(r_2).$$

Coefficients $C$ are obtained by diagonalising the target (FCHF) Hamiltonian

$$\langle \phi_f^{(\lambda)} | H_T | \phi_i^{(\lambda)} \rangle = \varepsilon_f^{(\lambda)} \delta_{fi}; \quad \lim_{N \to \infty} \sum_{n=1}^{N} |\phi_n^{(\lambda)}\rangle \langle \phi_n^{(\lambda)}| = I_T.$$
Convergent Close-Coupling theory

Target structure

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Hydrogen $\ell = 0$ energies for $\lambda = 1$ Laguerre bases
Projectile-target wavefunction is expanded as

\[ |\psi_i^{(+)}\rangle \approx I_T^{(N)}|\psi_i^{(+)}\rangle = \sum_{n=1}^{N} |\phi_n F_{ni}\rangle + \ldots \]  \hspace{1cm} (1)

Solve for \( T_{fi} \equiv \langle k_f \phi_f | V | \psi_i^{(+)} \rangle \) at \( E = \varepsilon_i + \epsilon_k \),

\[ \langle k_f \phi_f | T | \phi_i k_i \rangle = \langle k_f \phi_f | V | \phi_i k_i \rangle \]

\[ + \sum_{n=1}^{N} \int d^3k \frac{\langle k_f \phi_f | V | \phi_n k \rangle \langle k \phi_n | T | \phi_i k_i \rangle}{E + i0 - \varepsilon_n - \epsilon_k}. \] \hspace{1cm} (2)

Cross section: \( \sigma_{fi} \propto |\langle k_f \phi_f | T | \phi_i k_i \rangle|^2 \).
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- $e^-\text{-H total ionisation: } \sigma_{\text{ion}} = \sum_f \sigma_{fi} \text{ for } \varepsilon_f > 0$

![Graph showing cross section vs. total energy]
e^−-He(1^1S) ionisation

- e^−-He total ionisation: $\sigma_{\text{ion}} = \sum_f \sigma_{fi}$ for $\varepsilon_f > 0$

[Bray and Fursa, JPB 44, 061001 (2011)]
**e^−-N^{5+}(2^3S) ionisation**

**e^−-N^{5+} total ionisation:** \( \sigma_{\text{ion}} = \sum_f \sigma_{fi} \) for \( \varepsilon_f > 0 \)

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Positron scattering on molecular hydrogen

$e^+ - H_2$ collisions: total cross section

Photoionisation

**total single and double photoionisation of He**

![Graphs showing photoionisation cross sections for different processes.](image)

- $e^-$-H ionisation
- $e^-$-He-like atom/ion ionisation
- $e^+$-H$_2$

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Close-coupling methods “solve” quantum collision systems for one- and two-electron atomic targets:
- R-matrix with pseudostates (Bartschat, Badnell, )
- Time-dependent close-coupling (Pindzola, Colgan, )
- Convergent Close-Coupling (Fursa, Kadyrov, Bray, )

Considerable recent progress with light molecules
Complex atoms and molecules is a work in progress
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