The convergent close-coupling method for electron-atom scattering


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Introduction
Nonrelativistic CCC theory
Comparison with experiment
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1. Introduction
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   - Distant history
   - Recent history

2. Nonrelativistic CCC theory
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   - electron-atom scattering
   - convergence studies

3. Comparison with experiment
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   - electron-impact ionisation
   - proton-impact on hydrogen
The primary motivation is to provide accurate atomic collision data for science and industry:

- Astrophysics
- Fusion research
- Lighting industry
- Medical and materials applications

Provide a rigorous foundation for collision theory with long-ranged (Coulomb) potentials.
Introduction

Motivation

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

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Provide a rigorous foundation for collision theory with long-ranged (Coulomb) potentials.
Prior to the 1990s theory and experiment generally did not agree for:
- electron-hydrogen excitation or ionisation,
- electron-helium excitation or ionisation,
- single or double photoionisation of helium.

Consequently, we have been developing the convergent close-coupling (CCC) theory for electron/positron/photon/(anti)proton collisions with atoms/ions/molecules that is applicable at all energies for the major excitation and ionisation processes.
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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

Consequently, have developed a surface integral approach to scattering theory that is valid for short- and long-range potentials, see Kadyrov et al. PRL, 101, 230405 (2008) and Annals of Physics 324 1516 (2009).
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Structure: using the Laguerre basis $\xi_{nl}^{(\lambda)}(r)$ write:

- "one-electron" (H, Li, . . . , Cs) states:
  $$\phi_{nl}^{(\lambda)}(r) = \sum_{n'} C_{nl}^{n'} \xi_{n'l}^{(\lambda)}(r)$$

- "two-electron" (He, Be, . . . , Hg) 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

$$\langle \phi_f^{(\lambda)} | H_T | \phi_i^{(\lambda)} \rangle = \varepsilon_f^{(\lambda)} \delta_{fi}. \quad (1)$$
Hydrogen $\ell = 0$ energies for $\lambda = 1$ Laguerre bases

-0.1
-1
-10
-100
10
100
1000

energy (eV)

Laguerre basis size $N$
\[ \phi_\varepsilon^{(\lambda)}(r) \text{ for } N = 70, \lambda = 2 \text{ and } \phi_\varepsilon^{(R_0)}(r) \text{ for } R_0 = 134. \]
Scattering:

- **Electron-atom wavefunction is expanded as**

\[
|\psi_i^{(+)}\rangle \approx A \sum_{n=1}^{N} |\phi_n^{(\lambda)}\rangle \langle \phi_n^{(\lambda)} |\psi_i^{(+)}\rangle \equiv A l_N |\psi_i^{(+)}\rangle. \tag{2}
\]

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

\[
\langle k_f \phi_f^{(\lambda)} | T |\phi_i^{(\lambda)} k_i \rangle = \langle k_f \phi_f^{(\lambda)} | V |\phi_i^{(\lambda)} k_i \rangle \\
+ \sum_{n=1}^{N} \sum_{f} d^3 k \frac{\langle k_f \phi_f^{(\lambda)} | V |\phi_n^{(\lambda)} k \rangle \langle k \phi_n^{(\lambda)} | T |\phi_i^{(\lambda)} k_i \rangle}{E + i0 - \varepsilon_{n}^{(\lambda)} - \epsilon_k}. \tag{3}
\]

- **Have step-function behaviour**:

\[
\langle k_f \phi_f^{(\lambda)} | T |\phi_i^{(\lambda)} k_i \rangle \approx 0 \text{ for } \varepsilon_f^{(\lambda)} > \epsilon_k. 
\]
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\[ \langle k_f | V | \phi_i^{(\lambda)} \rangle = \langle k_f | V | \phi_i^{(\lambda)} \rangle \]

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Define scattering amplitude $f_{fi}$ via

$$
\langle \Phi_f^{(-)} | \underleftarrow{H - E} | \Psi_i^{(+)} \rangle \approx \langle k_f \phi_f^{(-)} | l_N (\underleftarrow{H - E}) A l_N | \psi_i^{(+)} \rangle
$$

$$
= \langle \phi_f^{(-)} | \phi_f^{(\lambda)} \rangle \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle,
$$

where $\varepsilon_f = \varepsilon_f^{(\lambda)}$ ensured $\langle \phi_f^{(-)} | l_N = \langle \phi_f^{(-)} | \phi_f^{(\lambda)} \rangle \langle \phi_f^{(\lambda)} |$.

- Discrete excitation $[\varepsilon_f < 0, \langle \phi_f^{(-)} | \phi_f^{(\lambda)} \rangle = 1]$:

$$
f_{fi}^{(N)}(k_f) = \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle,
$$

- Ionisation $[\varepsilon_f = q_f^2 / 2$, with $\langle \phi_f^{(-)} | \equiv \langle q_f^{(-)} |$]:

$$
f_{i}^{(N)}(q_f, k_f) = \langle q_f^{(-)} | \phi_f^{(\lambda)} \rangle \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle,
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$$= \langle \phi_f^{(-)} | \phi_f^{(\lambda)} \rangle \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle,$$

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Nonrelativistic CCC theory

- e⁻-H excitation and total ionisation (S-wave model)

![Graphs showing excitation and ionization cross sections for 1s, 2s, and 3s electrons in H atom.](image)

Poet 1978
CCC(30)
CCC(10)
CCC(5)

Cross section ($\pi a_0^2$) vs. projectile energy (eV)

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CCC method for electron-atom scattering
Nonrelativistic CCC theory

Comparison with experiment

atomic target structure
electron-atom scattering
convergence studies

- electron-impact excitation at 3 Ry

![Graphs showing cross section vs energy](image)

**Cross section** ($a_0^2$)

**Energy** (Ry)

- **Triplet**
  - CCC(10)
  - CCC(20)
  - CCC(30)

- **Singlet**
  - CCC(10)
  - CCC(20)
  - CCC(30)
electron-impact ionisation $\frac{d\sigma_i}{de}(e)$ at 3 Ry
Can estimate true SDCS from $\sigma_i^{\text{ion}}$ and $\frac{d\sigma_i}{de}(E/2)$.
54.4 eV e-H 2p angular correlation parameters

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Comparison with experiment

54.4 eV e-H 2p angular correlation parameters

Weigold, 1979
Williams, 1980

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CCC method for electron-atom scattering
54.4 eV e-H 2p angular correlation parameters

Comparison with experiment

- Electron-impact excitation
- Electron-impact ionisation
- Proton-impact on hydrogen

Weigold, 1979
Williams, 1980
CCC, 1992
Comparison with experiment

**54.4 eV e-H 2p angular correlation parameters**

- $P_1$
- $P_2$

Comparison with experiment:
- electron-impact excitation
- electron-impact ionisation
- proton-impact on hydrogen

Weigold, 1979
Williams, 1980
CCC, 1992
Crowe, 1996
21.8 eV e-Li 2p angular correlation parameters
21.8 eV e-Li 2p angular correlation parameters

![Graph of P₁ and P₂ angular correlation parameters](image)
20 eV e-Na spin asymmetries and spin-resolved $L_\perp$

![Graphs showing 20 eV e-Na spin asymmetries and spin-resolved $L_\perp$.](image)

- **A_{ex}(3S)**
- **A_{ex}(3P)**
- **$L_0^\perp$**
- **$L_1^\perp$**

Scattering angle (deg)

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CCC method for electron-atom scattering
**Comparison with experiment**

**e-H total ionisation cross section**

\[ \sigma_i = \int_0^E d\varepsilon \frac{d\sigma_i}{d\varepsilon}(\varepsilon). \]
25 eV e-H singly differential cross section $\frac{d\sigma_i}{de}(\varepsilon)$

![Graph showing the comparison between Shyn (1992), CCC(93), and CCC(\infty) for the singly differential cross section $\frac{d\sigma_i}{de}(\varepsilon)$ as a function of secondary energy $\varepsilon$ (eV).]
25 eV e-H doubly differential cross sections \( \frac{d^2\sigma_i}{dE d\Omega}(\theta) \)

- \( E_s = 2\text{eV} \)
- \( E_s = 3\text{eV} \)
- \( E_s = 4\text{eV} \)
- \( E_s = 5.7\text{eV} \)

- Shyn (1992)
- ECS
- CCC

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CCC method for electron-atom scattering
25 eV e-H $E_A = E_B = 5.7$ eV coplanar FDCS

- $\theta_{AB} = 80^\circ$
- $\theta_{AB} = 120^\circ$
- $\theta_{AB} = 100^\circ$
- $\theta_{AB} = 150^\circ$
e-Na $E_A = E_B$ eV coplanar fully differential Xsecs

- $E_A = E_B = 3$ eV
- $E_A = E_B = 5$ eV
- $E_A = E_B = 10$ eV
- $E_A = E_B = 15$ eV
- $E_A = E_B = 20$ eV
- $E_A = E_B = 30$ eV

scattering angle $\theta_A = -\theta_B$ (deg)
**e-H total ionisation cross section**

\[ \sigma_i = \int_0^E d\varepsilon \frac{d\sigma_i}{d\varepsilon} (\varepsilon). \]

- **1S**
  - Shah et al, JPB (1987)
  - CCC, PRL (1993)

- **2S**
  - Defrance et al, JPB (1981)
  - CCC, JPB (1997)
e-He total ionisation cross sections

1-1-S
exp, JPB(1984)
CCC, PRA(1995)

2-3-S
exp, JPB(1976)
CCC, JPB(2003)
CCC(S=0)
CCC(S=1)
exp, PRA(1989)
Comparison with experiment
electron-impact ionisation

- e-Li$^+$ total ionisation cross sections

![Graph showing ionisation cross sections vs projectile energy (eV)]

- Cross section ($10^{-18}$ cm$^2$)
- Projectile energy (eV)

- $0.87 \times 1$-1-S + $0.13 \times 2$-3-S


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Comparison with experiment

Electron-transfer cross section, CC(1,1) model

Total Cross Section (10^{-16} cm^2)

Incident Energy (eV/amu)

Newman [26] ○
Fite [27] □
Fite [28] ◊
Gealy [29] ▲
McClure [30] ▼
Bayfield [31] ▲
Wittkower [32] ▲
Hvelpland [33] ▲
Schwab [34] ▲
present ■
CDW2S [12] ▲

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Concluding remarks

- A general surface-integral approach to scattering theory has been formulated.
- There are (almost) no substantial discrepancies between CCC and experiment for:
  - electron-impact excitation or ionisation of quasi one- and two-electron targets
  - photon-impact single and double ionisation of He
- Presently we are extending CCC to:
  - positron collisions with quasi one- and two-electron targets
  - multi-channel proton collisions
  - more complicated targets, such as inert gases and molecules.

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