From Fully Differential Electron to Ion Impact Studies of Ionization: the Legacy of Don Madison

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Most important goal of atomic collision research: study quantum-mechanical few-body problem, one of the most fundamentally important and yet unsolved problems in physics.

Essence of FBP: Schrödinger equation not analytically solvable for more than two mutually interacting particles even if forces are precisely known. Particularly challenging: dynamic few-body systems like e.g. fragmentation processes.

Atomic fragmentation particularly suitable because:
- underlying interaction (electromagnetic) understood
- can select systems with small particle number ($\approx 3 - 5$)
Kinematically complete experiments
Where Don had to work on me (really hard and persistently): how to present results of a kinematically complete experiment on ionization

**Typical e,2e experiment:**
energy and angles of both final-state electrons measured **in coincidence**
⇒ FDCS usually presented as angular distribution of ejected electrons with all other parameters fixed.

**Typical ion-impact experiment:**
Earlier, either projectile scattering angle or electron spectra measured, but **not in coincidence**. With advent of COLTRIMS, electrons or projectiles measured **in coincidence with recoil ions**. ⇒ Usually, momentum distribution of various particles presented.

**Advantage of fully differential electron angular distribution:** more transparent
Often, structures in FDCS directly reflect interactions underlying reaction dynamics
Collision geometry and coordinate system

Blue: Scattering plane defined by $p_o$ and $p_f$

Red: electron emission plane defined by $p_o$ and $p_e$

Quantities fixed: $\phi_p = 0$, $\theta_p$, $\phi_e = 0$, and $E_e$, spectra plotted as a fct. of $\theta_e$

$q = p_o - p_f$
Experimental Setup, 75 keV p + He

Complete projectile and recoil-ion momenta measured. Electron momentum from conservation laws ⇒ **kinematically complete** ⇒ FDCS
Ionization of simple atoms or molecules by ion impact

Perturbative treatment: Born series

\[ T = \langle e^{ikr} \phi_f | V | e^{ikr} \phi_i \rangle + \langle e^{ikr} \phi_f | V G_0 V | e^{ikr} \phi_i \rangle + \]
\[ \langle e^{ikr} \phi_f | V G_0 V G_0 V | e^{ikr} \phi_i \rangle + \ldots \]

Distorted wave methods

Higher-order contributions treated in wavefunction of system

Break up three-body system into 3 two-body systems:

Continuum eigenstate of each two-body subsystem is a Coulomb-wave.

Approximation: Represent total wavefunction as product of three Coulomb terms

\[ \Psi_f = C_P e C_{PT} C_T \]

3C wavefunction ignores correlations between particle pairs \( \Rightarrow \) only accurate if one particle far from other two

In perturbation theory understanding few-body dynamics means describing relative importance of higher vs first-order contributions
One important higher-order process: post-collision interaction (PCI)

PCI maximizes for \( v_{el} = v_p \), for long time no kinematically complete data available!

\[ \frac{q_{el}}{q_p} = 0.34 \text{ mrad} \]

\[ E_{el} = 41.6 \text{ eV} \]
\[ \frac{v_{el}}{v_p} = 1.006 \]
75 keV $p + H_2$

Electrons ejected into scattering plane
$\theta_p = 0.55$ mrad

$e = 50$ eV
$e = 53$ eV
$e = 57$ eV
$e = 60$ eV

M. Dhital et al.
PRA 99, 062710 (2019)
75 keV p + H$_2$

Scattering plane
Electron energy = 30 eV

\[ FDCS (cm^2 s eV) \]

\[ \theta_p = 0.1 \text{ mrad} \]

\[ \theta_p = 0.2 \text{ mrad} \]

\[ \theta_p = 0.325 \text{ mrad} \]

\[ \theta_p = 0.55 \text{ mrad} \]
Discrepancies between experiment and between two conceptually very similar theoretical models, which appear to maximize near velocity matching and at large $\theta_p$

In these regions FDCS particularly sensitive to details of few-body dynamics!

Possible causes for discrepancies:

a) **3C wavefunction inaccurate** if all particles close together. PE – PT – PE sequence selects such events.

b) **Capture channel not included** in theory $\Rightarrow$ due to unitarity capture is erroneously counted as ionization in transition amplitude

Both problems addressed by non-perturbative approaches such as **WP-CCC**. Calculations currently in progress $\Rightarrow$ Alisher Kadyrov
$p + He$

$\varepsilon = 65.5 \text{ eV} \ (v_{el}/v_p = 1) , \ \theta_p = 0.5 \text{ mrad}$

2 signatures of PCI:

a) forward peak

b) forward shift of binary peak

Next project: go as far away as possible from $v_{el}/v_p = 1$ in order to suppress PCI.

Should enable us to study non-PCI higher-order effects.

Use signatures of PCI as monitor for residual PCI contributions
\( \varepsilon = 25.6 \text{ eV} \)

One PCI signature, forward peak, completely absent

Arrows indicate direction of momentum transfer
\( \varepsilon = 100 \text{ eV} \)

Compared to \( \frac{v_{\text{el}}}{v_p} = 1 \), forward peak strongly suppressed, but compared to \( \frac{v_{\text{el}}}{v_p} \ll 1 \) a significant residue remains.
K.H. Spicer et al.,
PRA 104, 052815 (2021)
Forward shift is larger at $\varepsilon = 25.6$ eV, but ...
Schulz et al. PRA 88, 022704 (2013): projectile – target nucleus interaction can also lead to forward shift.

2 components to forward shift, one contributes only at $v_{el}/v_p < 1$, the other only near and above $v_{el}/v_p = 1$.

Forward shift for $\varepsilon = 100$ eV caused mostly by PCI, but for $\varepsilon = 25.6$ eV mostly due to non-PCI effects?
Conclusions

- FDCS for ionization measured for a broad range of electron energies

- Near velocity matching PCI signatures: a) forward peak b) forward shift of binary peak

- Forward peak absent far below, but residue remains far above matching velocity

- Not every forward shift of binary peak is signature of PCI
  - far below matching velocity non PCI higher-order effects
  - above matching velocity mostly due to PCI

- Without Don Madison and his distorted wave calculations we would not be where we are. But now non-perturbative calculations needed.