Fully Differential Study of Post-Collision Effects in Ionization of H$_2$ by Proton Impact

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Quantum-mechanical few-body problem one of the most fundamentally important, unsolved problems in Physics!

Schrödinger equation not solvable for more than two particles, even when underlying forces are precisely known

Dynamic few-body systems like fragmentation processes

Atomic fragmentation particularly suitable because:
- underlying interaction (electromagnetic) understood
- can select systems with small particle number
  \(\approx 3 - 5\) \(\Rightarrow\) kinematically complete experiments
Ionization of H\textsubscript{2} by p impact

Perturbative treatment: expand T in powers of interaction potential V (Born series)

\[ T = \langle e^{ik_f} \phi_f \mid V \mid e^{ik_i} \phi_i \rangle + \langle e^{ik_f} \phi_f \mid VG_0V \mid e^{ik_i} \phi_i \rangle + \]

\[ < e^{ik_f} \phi_f \mid VG_0VG_0V \mid e^{ik_i} \phi_i > + \ldots \]

In perturbation theory understanding few-body dynamics means describing relative contributions of higher- vs first-order terms

Particularly important higher-order process: PCI

PE – ET – PE sequence

PE – PT – PE sequence
Alternative to Born Series: Distorted wave methods

Higher-order contributions treated in wavefunction of system
Break up three-body system into 3 two-body systems:

The continuum eigenstate of each two-body subsystem is a (distorted) Coulomb-wave. Approximation: Represent total wavefunction as product of three Coulomb-waves

\[ \Psi_f = C_{Pe}C_{PT}C_{Te} \]

Conceptually, all interactions treated to all orders, but 3C wavefunction ignores correlations between particle pairs \( \Rightarrow \) only accurate if one particle far from other two \( \Rightarrow \) at small distances none of higher-order terms described accurately

PCI maximizes for \( v_{el} = v_p \), no kinematically complete data available!
Complete projectile and recoil-ion moment measured. Electron momentum from conservation laws ⇒ **kinematically complete** ⇒ FDCS
Three-Dimensional Fully Differential Single Ionization Data

Blue: Scattering plane defined by \( p_o \) and \( p_f \)

Red: electron emission plane defined by \( p_o \) and \( p_e \)

Quantities fixed: \( \phi_p = 0 \), \( q \), \( \phi_e = 0 \), and \( E_e \), spectra plotted as a function of \( \theta_e \)
Results: FDCS 75 keV p + H₂

ε = 53 eV, θₚ = 0.1 mrad

ε = 60 eV, θₚ = 0.55 mrad

small θₚ:
a) direction of q much closer to θₑl = 0
b) binary peak much weaker
⇒ only single peak

„forward peak“ signature of PCI projectile and electron attract each other towards beam axis

„binary peak“ signature of 1ˢᵗ order process momentum conservation: near θₚ
FDCS for $\theta_p = 0.1$ mrad

Red curves: 3DW model
Blue curves: CDW-EIS model
$\theta_p = 0.2 \text{ mrad}$

The diagrams show the FDCS (cm$^2$/sr/eV) as a function of $\theta_{el}$ (deg) for different energies $\epsilon$.

- $\epsilon = 50 \text{ eV}$
- $\epsilon = 53 \text{ eV}$
- $\epsilon = 57 \text{ eV}$ (with $v_{el} = v_p$)
- $\epsilon = 60 \text{ eV}$

The plots demonstrate the variation of the differential cross section with the electron scattering angle $\theta_{el}$ for various electron energies.
$\theta_p = 0.325$ mrad

$\varepsilon = 50$ eV

$\varepsilon = 53$ eV

$\varepsilon = 57$ eV

$\varepsilon = 60$ eV

$\varepsilon = 50$ eV

$\varepsilon = 53$ eV

$\varepsilon = 57$ eV

$\varepsilon = 60$ eV

$\theta_e (\text{deg})$

$\theta_\text{el} (\text{deg})$

$\theta_p = 0.325$ mrad
\( \theta_p = 0.55 \text{ mrad} \)
Energy-dependence of FDCS for $\theta_e = 0^\circ$

![Graphs showing energy-dependence of FDCS for different values of $\theta_p$.](image-url)
Large discrepancies between experiment and between two conceptually very similar theoretical models!

At small electron energies much smaller discrepancies and theories agree with each other ⇒ at velocity matching FDCS particularly sensitive to details of few-body dynamics!

Possible causes for discrepancies:

a) PT interaction not accurate in theory
   3C wavefunction only accurate if at least 1 particle far from other 2. PE − PT − PE sequence selects events where all 3 particles are close to each other

b) Capture channel not included in theory ⇒ due to unitarity capture is erroneously counted as ionization in transition amplitude

c) Projectiles treated as fully coherent waves, but in reality due to intrinsic momentum spread coherence length is finite
What type of theory is needed?

a) **non-perturbative** because slow projectiles cannot be regarded as small perturbation ⇒ large basis set needed

b) should incorporate **two-center basis set** including bound projectile states to account for capture

c) projectiles should be described by **wave packet** with a width reflecting the **coherence length**

Non-perturbative models with two-center basis sets for ion impact have been developed recently (Kadyrov et al., Walters et al., Pindzola et al.). First results on FDCS for H₂ can be expected soon.

Incorporating wave packets in such models very challenging
Conclusions

• Fully differential cross sections for ionization in 75 keV p + H$_2$ measured.

• Major discrepancies between experiment and theory and between two conceptually very similar models.

• At matching velocity FDCS very sensitive to details of few-body dynamics.

• Potential problems with perturbative methods:
  a) capture not included
  b) 3C wavefunction not accurate when all particles close
  c) projectile coherence not realistically described

• What is needed: non-perturbative calculations with two-center basis set and wave packet describing projectile.
SBA-2C:
Black: FBA no PCI
Blue: only PE-ET-PE
Red: PE-ET-PE and PE-PT-PE

⇒ PE – ET – PE sequence dominant PCI channel in SBA-2C

CDW-EIS:
Black: FBA no PCI
Blue: only PE-ET-PE
Red: PE-ET-PE and PE-PT-PE

⇒ PE – PT – PE sequence dominant PCI channel in CDW-EIS