Fully Differential Studies of Atomic Collision Processes

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What is a fully differential cross section (FDCS)?

Consider process:

$$X^{q+} + A \rightarrow X^{q'+} + A^{Q+} + ne^{-}$$

n+2 independently moving particles in final state

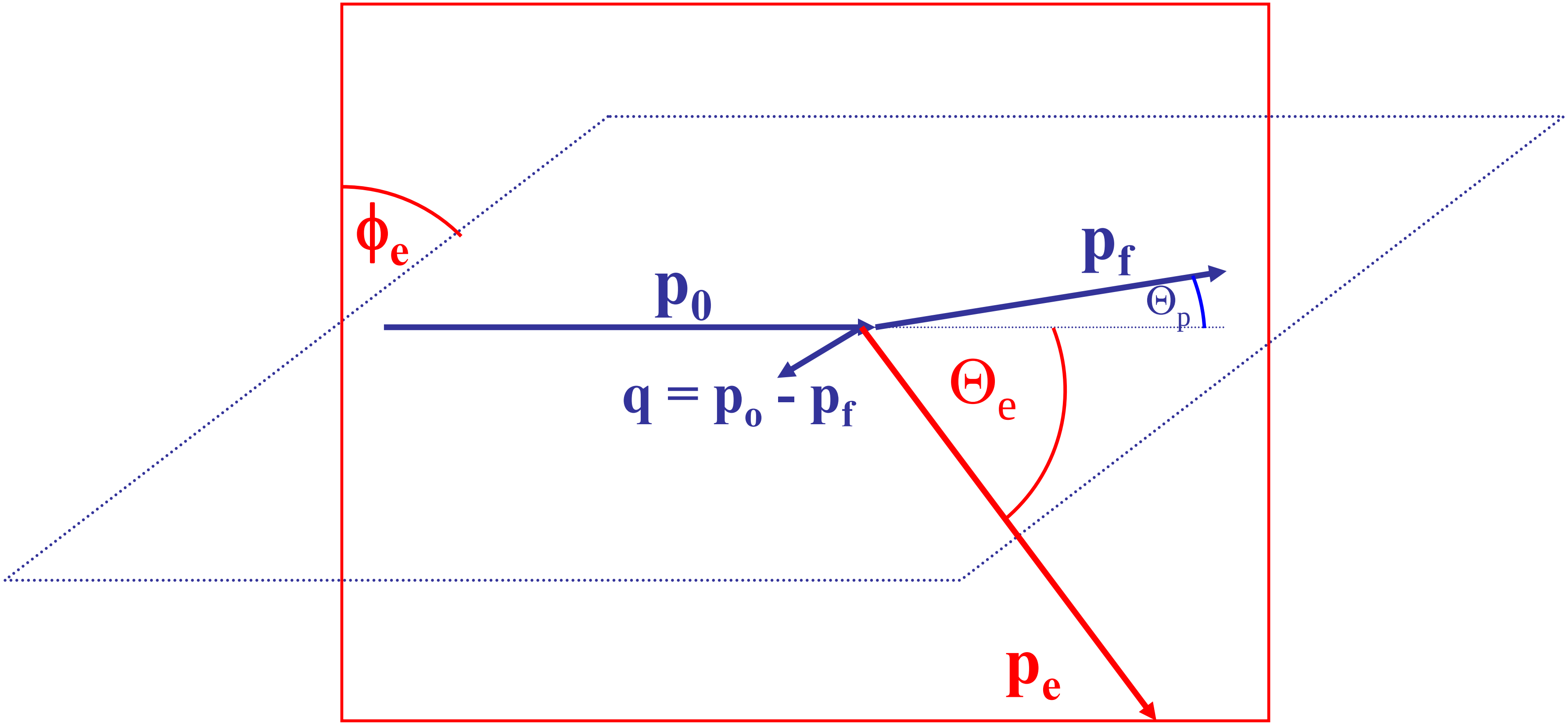
kinematics complete: 3(n+2) momentum components

Conservation laws: 3(n+2) – 4 components independent

E.g. Single ionization, n = 1 ⇒ 5 indpendent components

⇒ FDCS = fivefold differential cross section

Double ionization: FDCS = eightfold differential etc.



Blue: Scattering plane defined by p_o and p_f

Red: electron emission plane defined by p_o and p_e

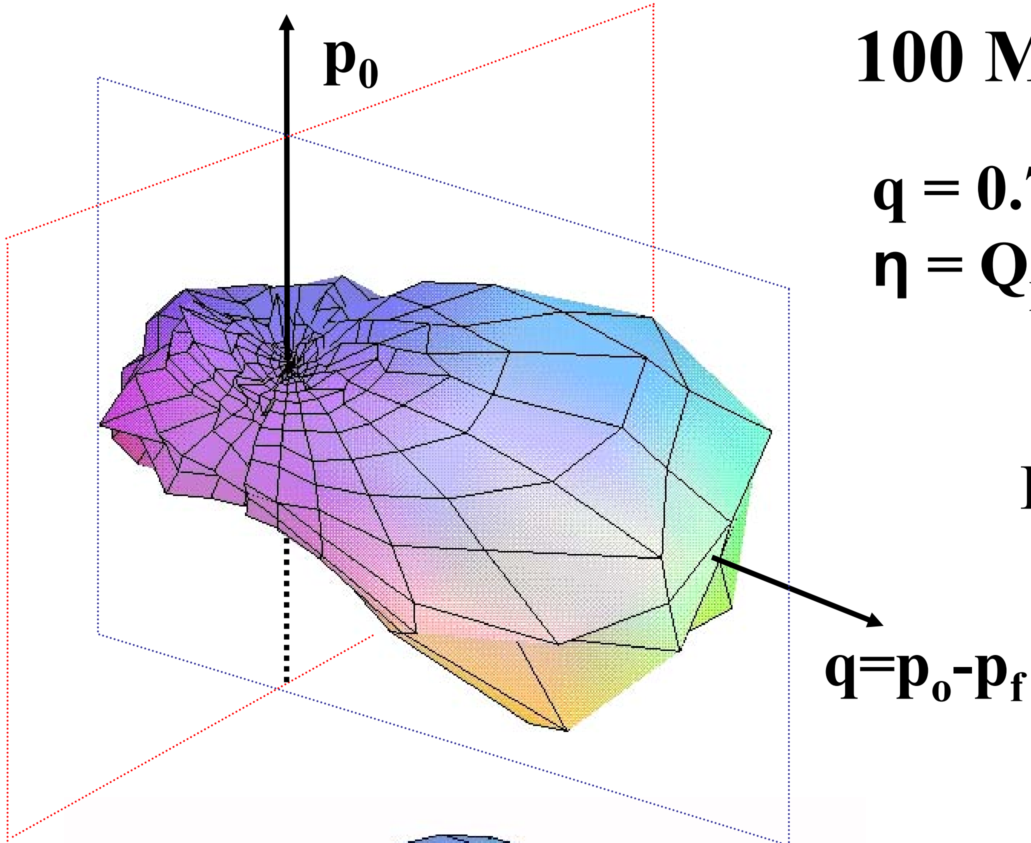
Quantities fixed: ϕ_p, q, and E_e Spectra plotted as a fct. of ϕ_e and θ_e

⇒ 5 independent components determined ⇒ FDCS

100 MeV/amu C^{6+} + He

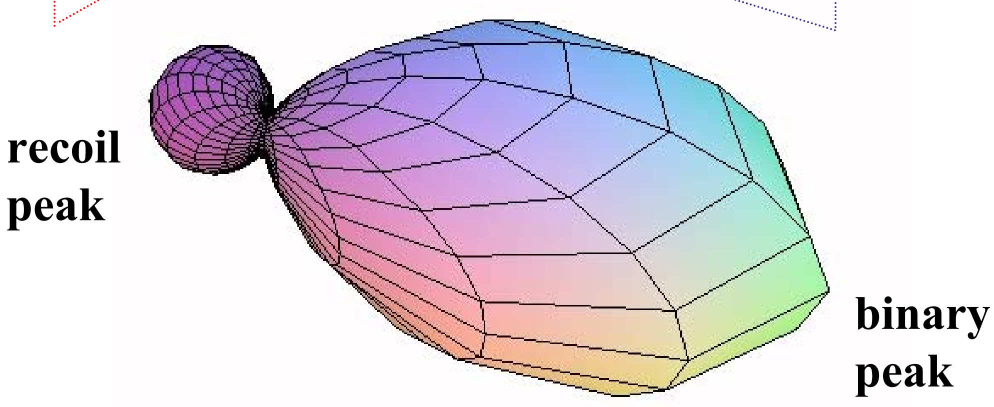
$q = 0.75$ a.u. $E_e = 6.5$ eV

$\eta = Q_p/v_p = 0.1$



Experiment

Schulz et al.
Nature 422, 48, 2003



Theory
(3DW, Madison)

Discrepancies due to elastic scattering of proj. off target nucleus

I) Demonstrate that data now qualitatively understood

II) Introduce new analysis technique which opens new possibilities, both for experimental and theoretical analysis: Event Generator Method

a) Convolution of theory with exp. resolution in multi-dimensional space, inaccessible previously

⇒ direct comparison exp.-theory becomes possible

b) Theory can be convoluted with physics effects not included in original calculation

c) Any measurable cross section can be computed. Not always possible with conventional methods because of lack of symmetry

Event Generator Technique (example SI)

1.) Choose 5 momentum components using random generator

2.) For this set calculate FDCS with theoretical model of choice

3.) Use Monte Carlo method to decide, based on calculated FDCS, whether to store event in file or to reject

4.) Repeat 1. to 3. until event file of „good“ ionization events with sufficient statistics is generated (typically ≈ 1 M events)

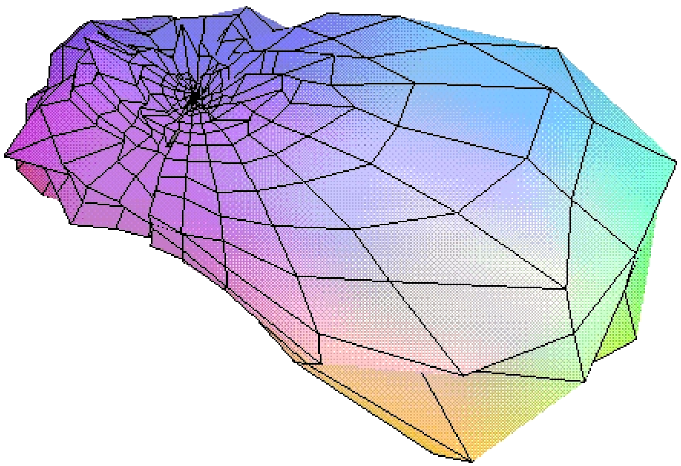
Convolution with resolution or physics

Simply add to each momentum component appropriate resolution event-by-event or
e.g. elastic scattering: add to components of q and recoil momentum the momentum transfer occuring in elastic scattering

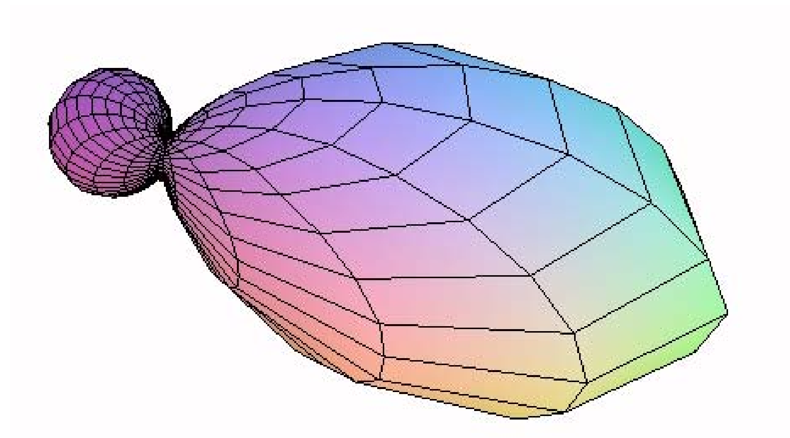
100 MeV/amu C^{6+} + He, fully differential angular e^{-} - distribution

E_e = 6.5 eV, q = 0.75 a.u.

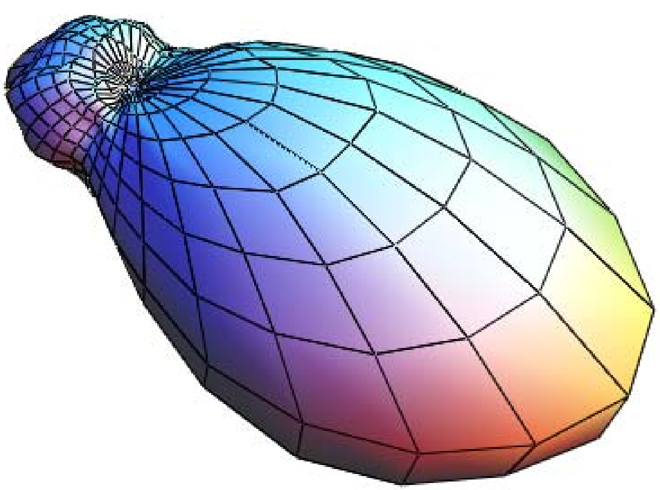
Experimental data



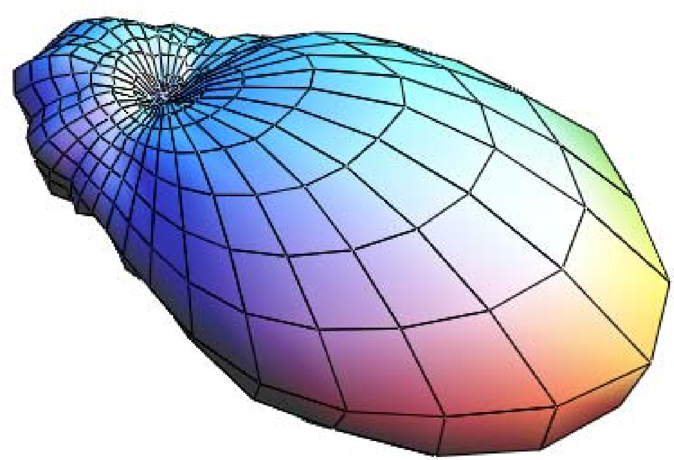
FBA, unconvoluted



FBA, convoluted with elastic scattering



FBA, convoluted with elastic scattering and resolution



FDCS very sensitive test of theoretical models

BUT important <u>drawback:</u>

FDCS covers only tiny fraction of total cross section

typically plotted as a function only one particle

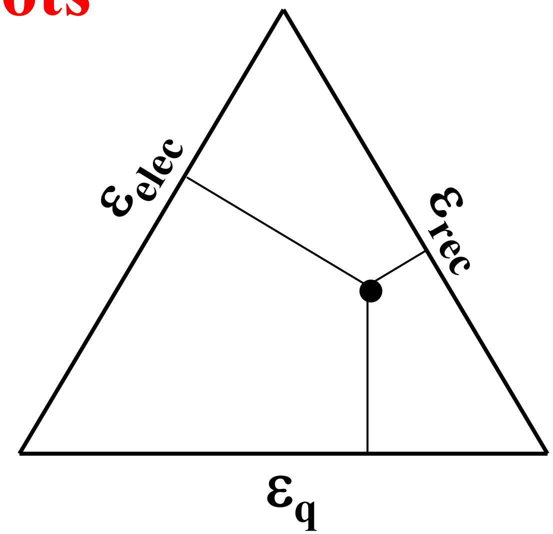
⇒FDCS do not provide comprehensive picture of reaction dynamics

Solution:
Dalitz-plots

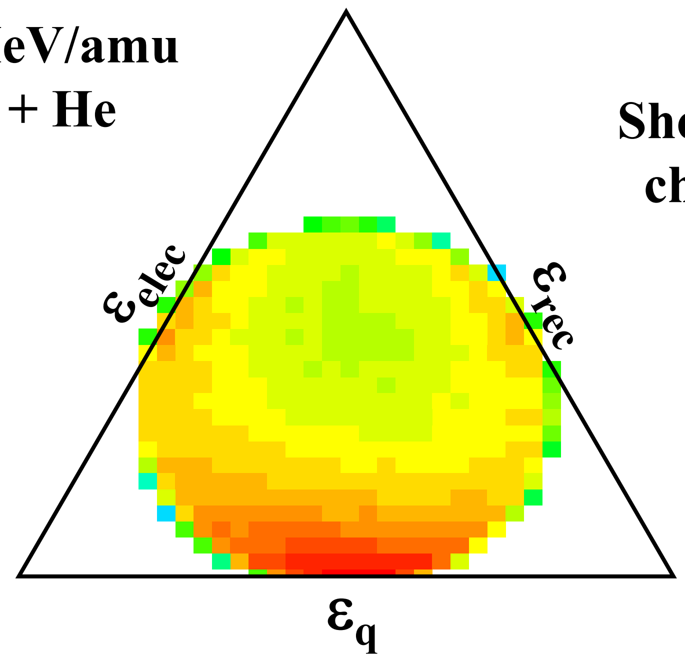
Coordinates:

$\varepsilon_i = p_i^2/(\Sigma p_j^2)$,
i,j = q, electron, recoil-ion

ε_i is proportional to distance from respective triangle side



3.6 MeV/amu
Au^{53+} + He



Shows momentum exchange between all three particles simultaneously. Dominated by "internal target" correlation

Four-particle break-up processes:
Conventional Dalitz plots present data only for three particles
$\Rightarrow$ only feasible if fourth particle is integrated over

Here, we introduce generalization of Dalitz plots to four particles

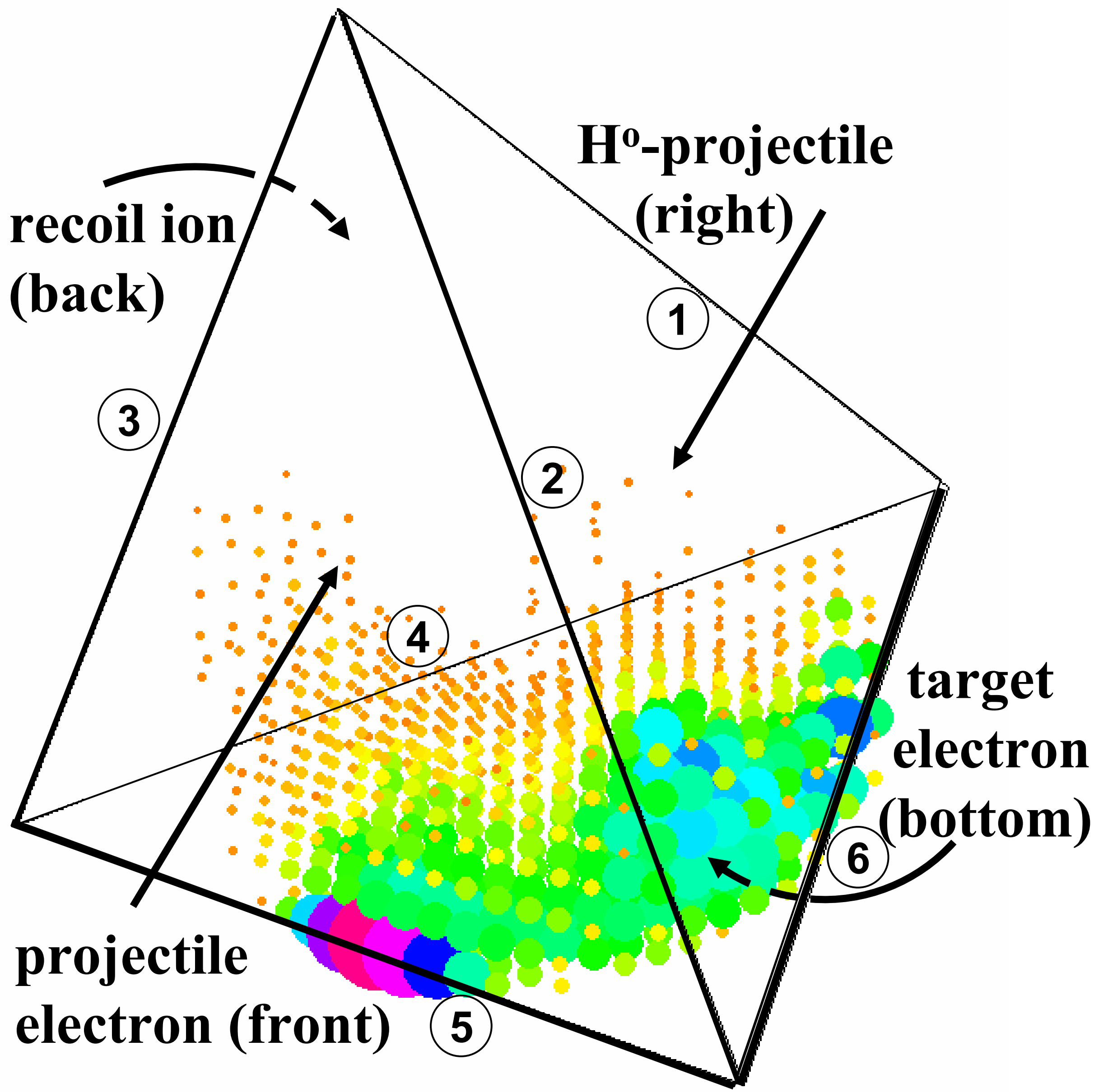
Same basic idea: relative squared momenta of all fragments ε_i are plotted. Equilateral triangle is replaced by tetrahedron (i.e. three-dimensional coordinate system)

For a given data point the ε_i of the four particles are given by the perpendicular distances to the four tetrahedron planes.

First example: 200 keV $H^- + He \rightarrow H^o + He^+ + 2e^-$

Binary interactions

1. electron – electron
2. recoil – target elec.
3. H^0 – target electron
4. H^0 – project. electr.
5. H^0 – recoil
6. recoil – project. elec.



First example: 200 keV $H^- + He \rightarrow H^o + He^+ + 2e^-$

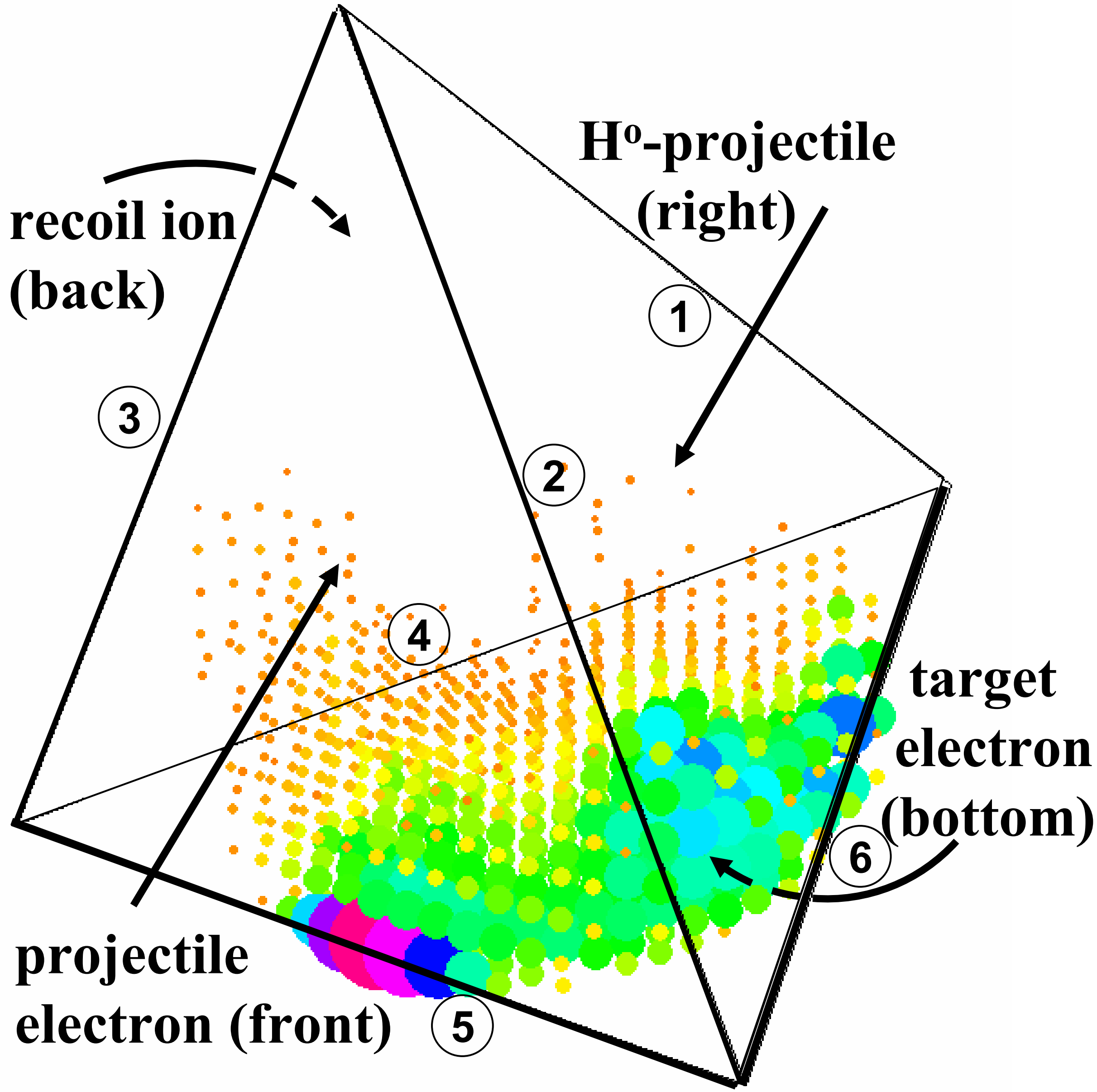
Observations:

1.) Binary electron-electron interaction (1) surprisingly weak

2.) Momentum exchange dominated by elastic scattering between cores (5)

3.) "Internal" correlation of each electron with corresponding core (2 and 4) much weaker than in single ionization, especially projectile

4.) Pronounced binary interaction He^+ - projectile electron (6), but weak for H^o – target electron (3)



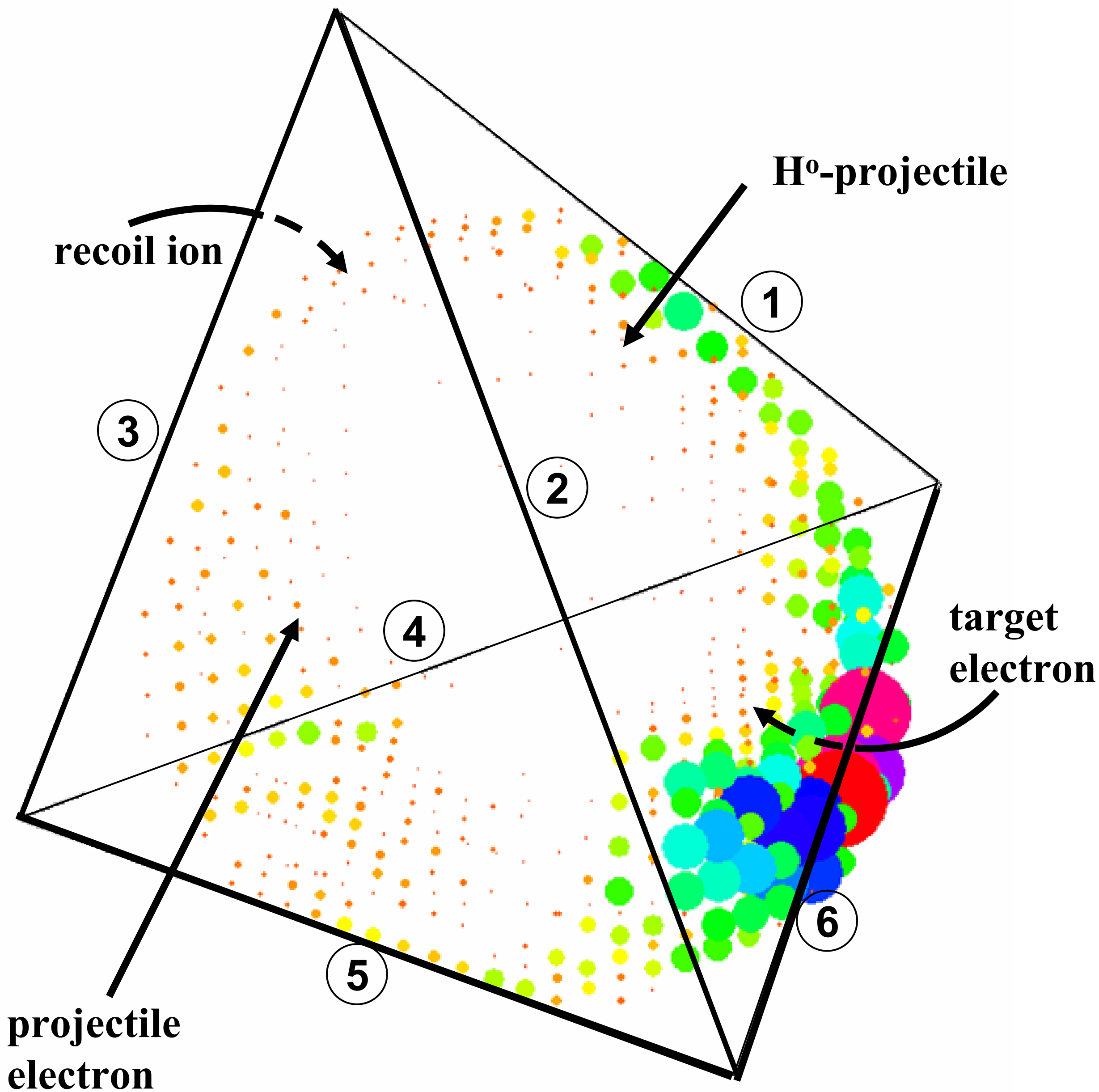
<u>Longitudinal</u> momentum components $H^- + He \rightarrow H^o + He^+ + 2e^-$

<u>Very different behavior:</u>

1.) Binary recoil – projectile electron interaction (6) dominant

2.) elastic He^+ - H^o scattering (5) insignificant

3.) Some contribution from binary electron-electron interaction (1), i.e. first order, now visible



FDCS nevertheless crucially important to test theory

Problem for multiple-electron transitions:

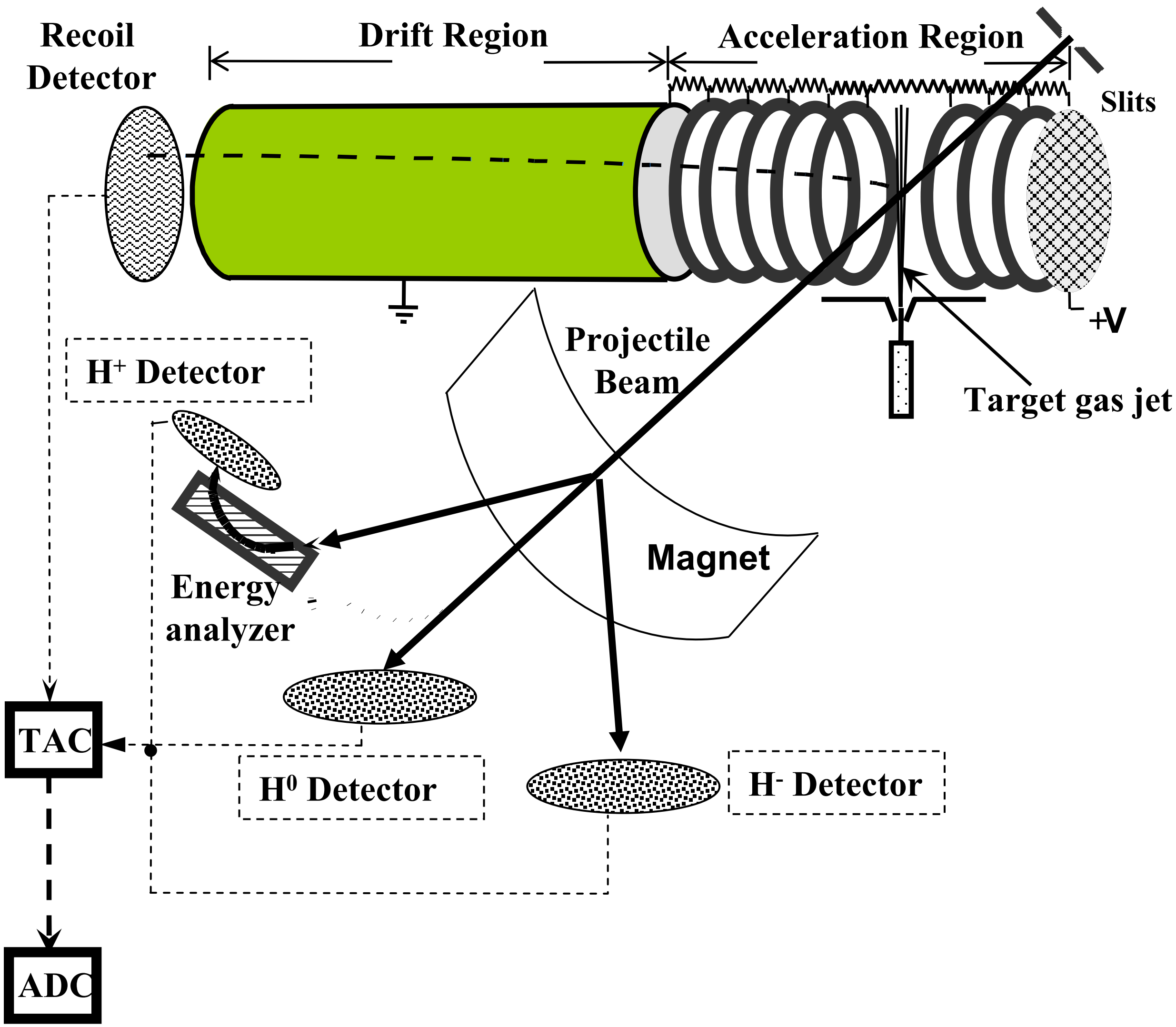
a) Cross sections orders of magnitude smaller than for one-electron transitions

b) Multiple ionization: degree of differentiality of FDCS increases with number of continuum electrons

Alternative: Transfer-excitation $p + He \rightarrow H + He^{+*}$

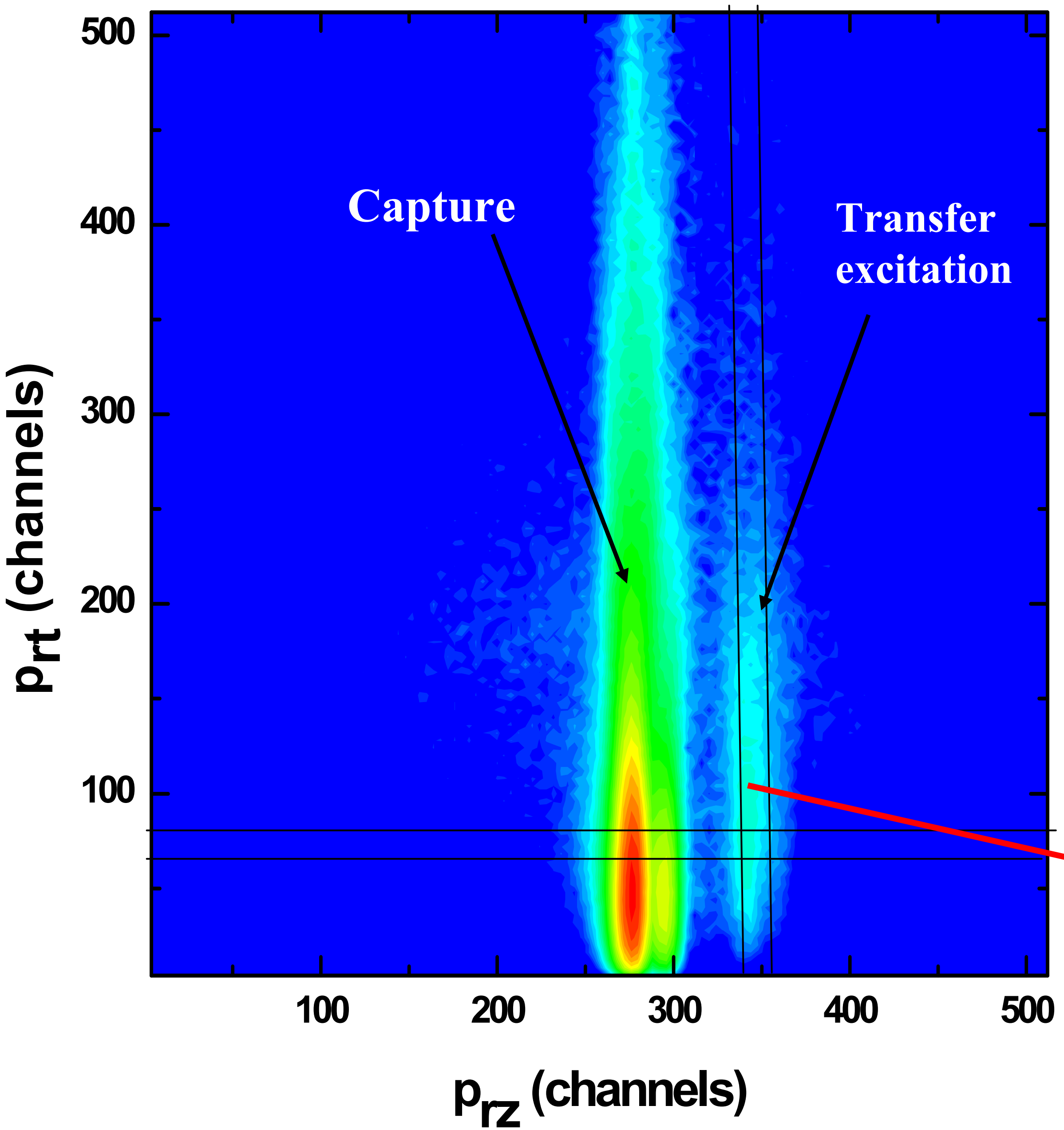
No continuum electrons $\Rightarrow d^2\sigma/d\theta d\phi \sim d\sigma/d\Omega(\theta)$ readily constitutes FDCS

Rolla Reaction Microscope



Coincidences between fully momentum analyzed He^{+} ions and neutralized projectiles

Coincident recoil-ion momentum spectrum



- **Longitudinal:**

  From conservation laws

  $p_{rz} = - Q/v_o - v_o/2$

$\Rightarrow$ long. recoil momentum directly reflects Q-value

$\Rightarrow$ use p_{rz} to identify process.

- **Transverse:**

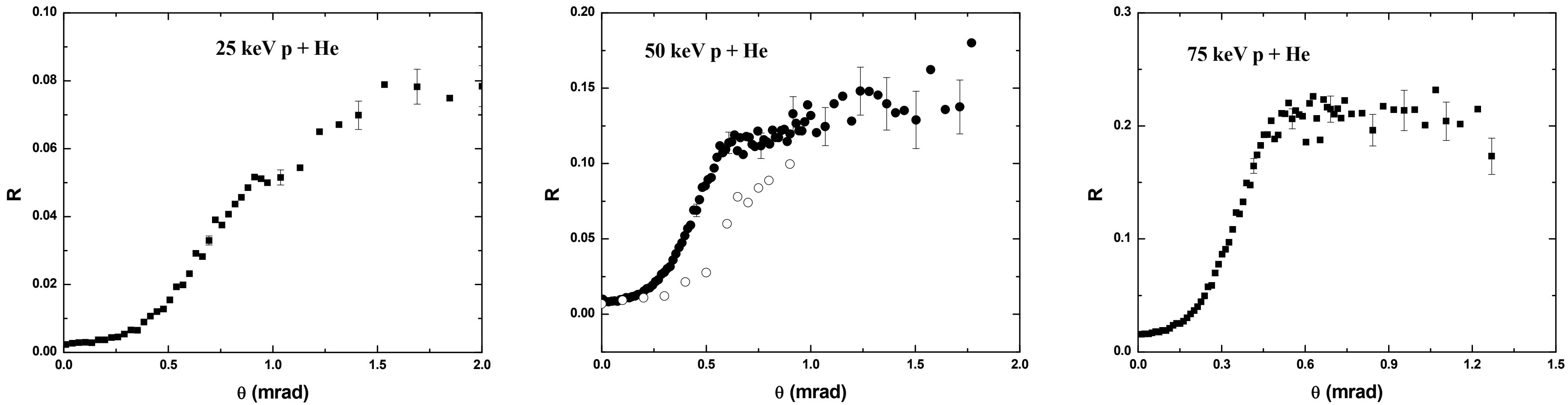
  $p_{rt} = p_{pt} = p_o \sin\theta$

$\Rightarrow$ transv. recoil momentum yields scatt. angle

$\sim d\sigma/d\theta$ and

$d\sigma/d\Omega = (d\sigma/d\theta)/2\pi \sin\theta$

In case of double ionization, transfer-ionization and double excitation ratios to one-electron process were analyzed to study $e^- - e^-$ interaction. Here: $R(\theta) = d\sigma_{TE}(\theta)/d\sigma_{SC}(\theta)$



Independent electron model (IEM):

Transfer Excitation: $d\sigma/d\Omega_{TE}=2P_{SE}P_{SC}d\sigma/d\Omega_{el}$

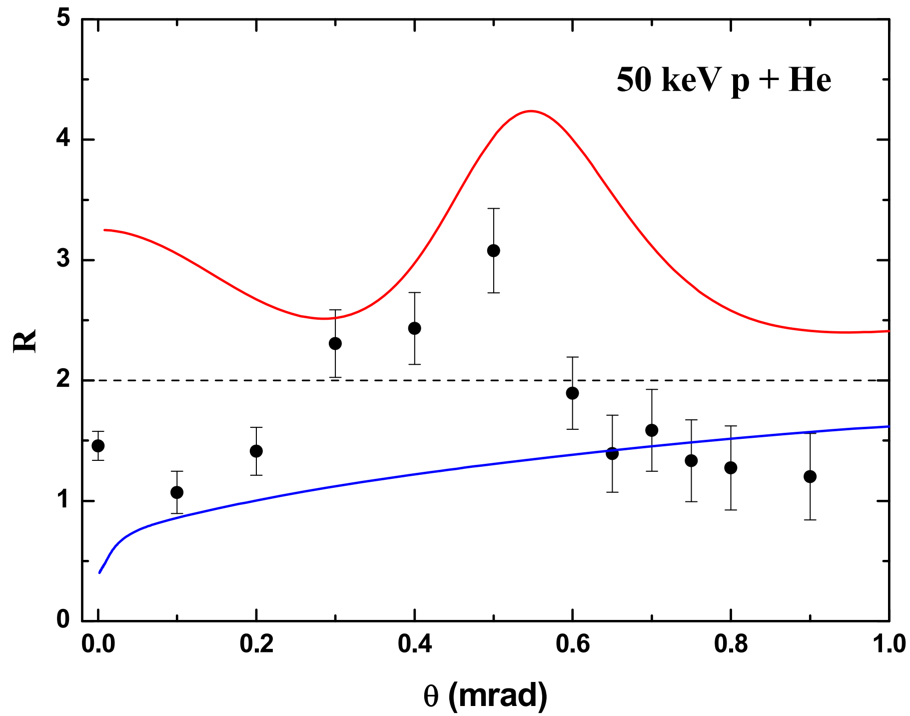
Double Excitation $d\sigma/d\Omega_{DE}=P_{SE}^2\, d\sigma/d\Omega_{el}$

Single Excitation $d\sigma/d\Omega_{SE}=P_{SE}\, d\sigma/d\Omega_{el}$

Single capture $d\sigma/d\Omega_{SC}=P_{SE}d\sigma/d\Omega_{el}$

$\Rightarrow R_{TE} = 2R_{DE} = 2P_{SE}(\theta)$ $\Rightarrow R = R_{TE}/R_{DE} = 2$

Double ratio R_{TE}/R_{DE}



Black dashed curve: IEM

Blue solid curve: BGM with classical treatment of elastic scattering (BGM-CL)

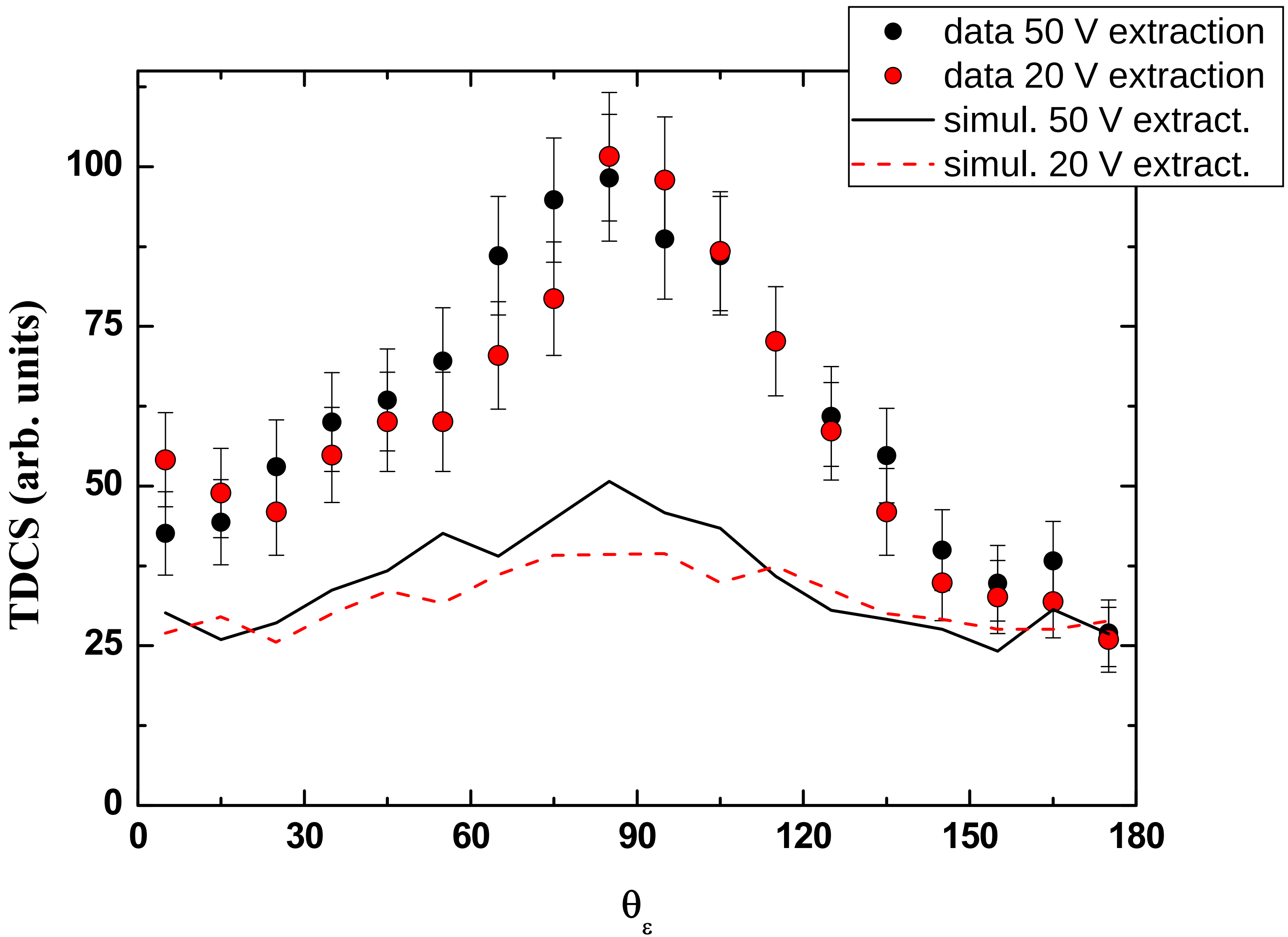
Red solid curve: BGM with quantum-mechanical treatment of el. scattering, includes dynamic coupling between electronic transition and nucl. motion (BGM-QM)

Only BGM-QM qualitatively reproduces peak structure

⇒Structure probably related to quantum-mechanical nature of elastic scattering and/or dynamic couplings, not to e^- - e^- interaction

Conclusions

- **FDCS crucially important for sensitive tests of theory**
- **Event Generator Technique very powerful tool for experimental and theoretical analysis**
- **4-particle Dalitz plots very powerful to visualize complete four-body dynamics without loss of any part of total cross section**
- **FDCS for transfer-excitation can qualitatively only be described if elastic scattering is treated quantum-mechanically**


data 50 V extraction
data 20 V extraction
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TDCS (arb. units)
0
25
50
75
100
0
30
60
90
120
150
180
θ_ε