3-Body and 4-Body Atomic Collisions Theory (The most boring title ever)

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XSEDE
Extreme Science and Engineering Discovery Environment
NSF

My Story (short version)

DEPARTMENT OF PHYSICS
Illinois State University

STATE
YOUR TRAJECTORY.

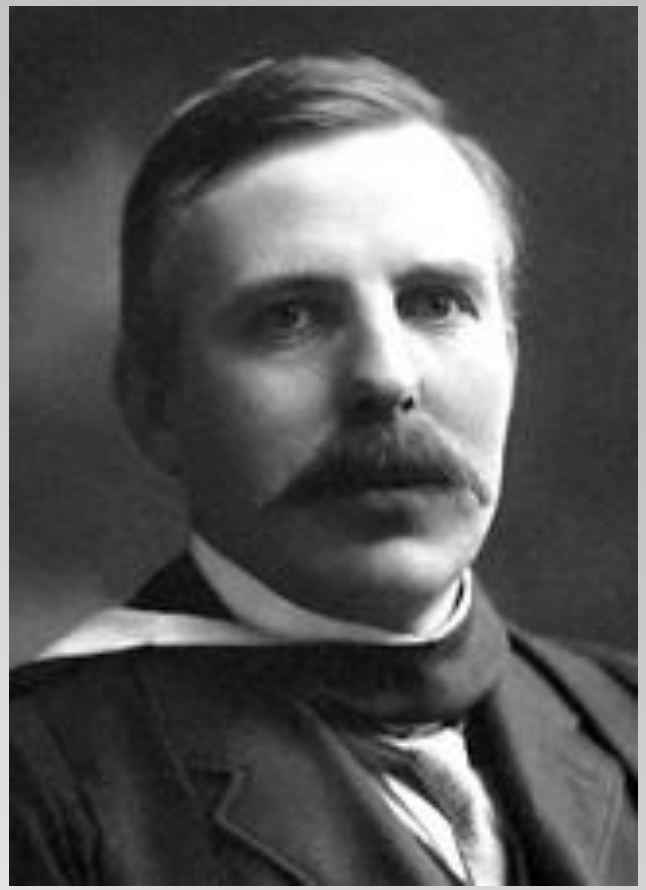
- 130 majors
- 18 grads per year
- 11 faculty
- 4 degree sequences
  - Physics
  - Computational Physics
  - Physics Engineering
  - Physics Teacher Education

Atomic Collisions

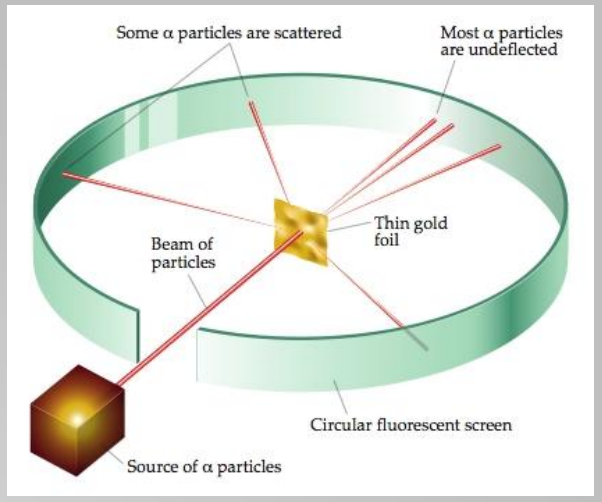
Atomic Collisions

- A very short historical Perspective

Ernest Rutherford



- Nobel Prize in Chemistry (1908) "*for his investigations into the disintegration of the elements, and the chemistry of radioactive substances*"
- Gold Foil Experiment (1908-1913)



Classical Picture

Atomic collisions are governed by Quantum Mechanics

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

- Goal is to understand about atomic structure and few-particle interactions
- If we know Ψ, we know everything
- Problem is that we don't know Ψ, and often times can't find Ψ

Atomic Collisions

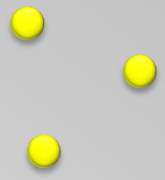
- Underlying problem

- Force governing collisions is known
  - Coulomb Force
  - Two body problem

$$F = \frac{kq_1q_2}{r^2}$$

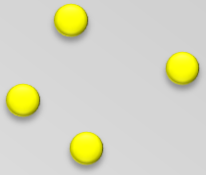
➡ Analytical solution

- Three body problem



➡ Numerical solution

- Four body problem



➡ No solution, Much to learn, difficult

- Five body problem

  Ask Nate Harshman!!!

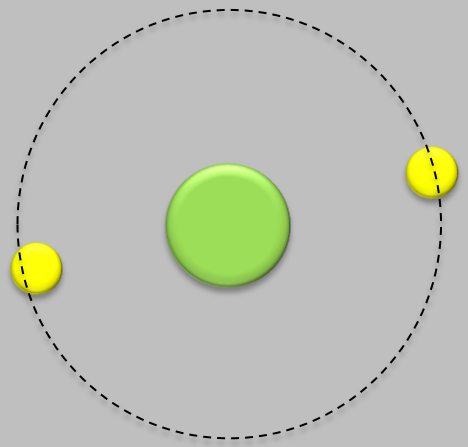
Atomic Collisions

- Problems of Interest - Ionization
  - Frozen Core Approximation
  - Out-of-Plane Collisions

4-Body Collisions
Ionization

Frozen Core 3-Body Model

- Helium atom approximated as 1-electron atom
- Core consists of nucleus and inactive electron



Single Ionization – Frozen Core 3-Body Model

- Used successfully for decades
- Significantly simplifies calculations

“Problem”:

Helium has 2 electrons

What effect does the second, “inactive” electron have on the cross section?

The Models – Perturbation Theory Fully Differential Cross sections

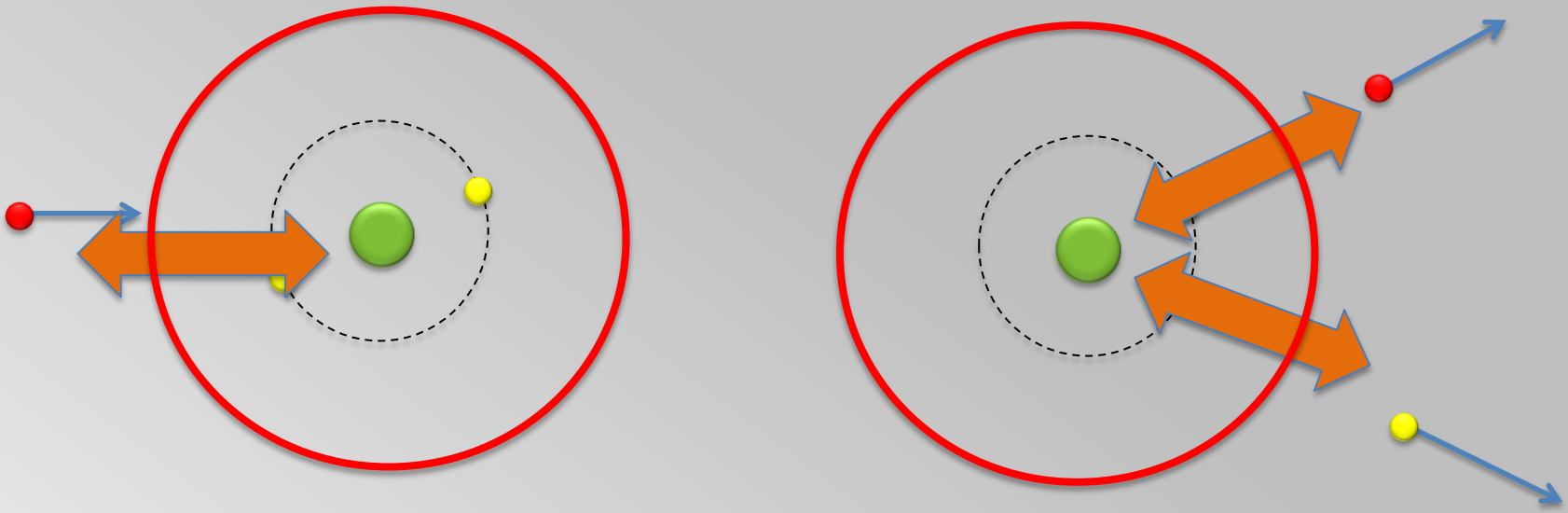
- Position and momentum of all particles before and after collision known (or measured).

$$FDCS \propto |T|^2 \qquad T = \langle \psi_f | V | \psi_i \rangle$$

The Models

4-body model

$$T = \left\langle \chi_f^{proj}\, \chi_{e_1}^{ejected}\, \xi_{e_2}^{bound} \middle| V^{4-body} \middle| \chi_i^{proj}\, \Phi_{e_1,e_2}^{helium} \right\rangle$$



The Models

3-body model

$$T = \left\langle \chi_f^{proj} \chi_{e_1}^{ejected} \left| V^{3-body} \right| \chi_i^{proj} \varphi_{e_1}^{helium} \right\rangle$$

3-BODY AND 4-BODY MODEL DIFFERENCES

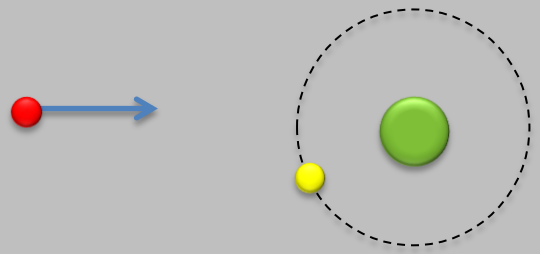
1. Initial state helium atom wave functions

   3-body

   1 e^- wf

   4-body

   2 e^- wf with correlation

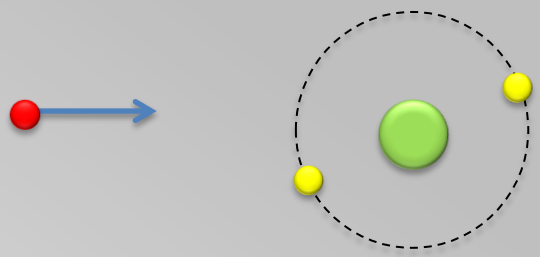


3-body

2. Initial state interaction potentials are different

   3-body $$V = -\frac{1}{r_p} + \frac{1}{r_{pe}}$$

   4-body $$V = -\frac{2}{r_p} + \frac{1}{r_{pe_1}} + \frac{1}{r_{pe_2}}$$



4-body

3-BODY AND 4-BODY MODEL DIFFERENCES

3. Final state He^+ wave functions

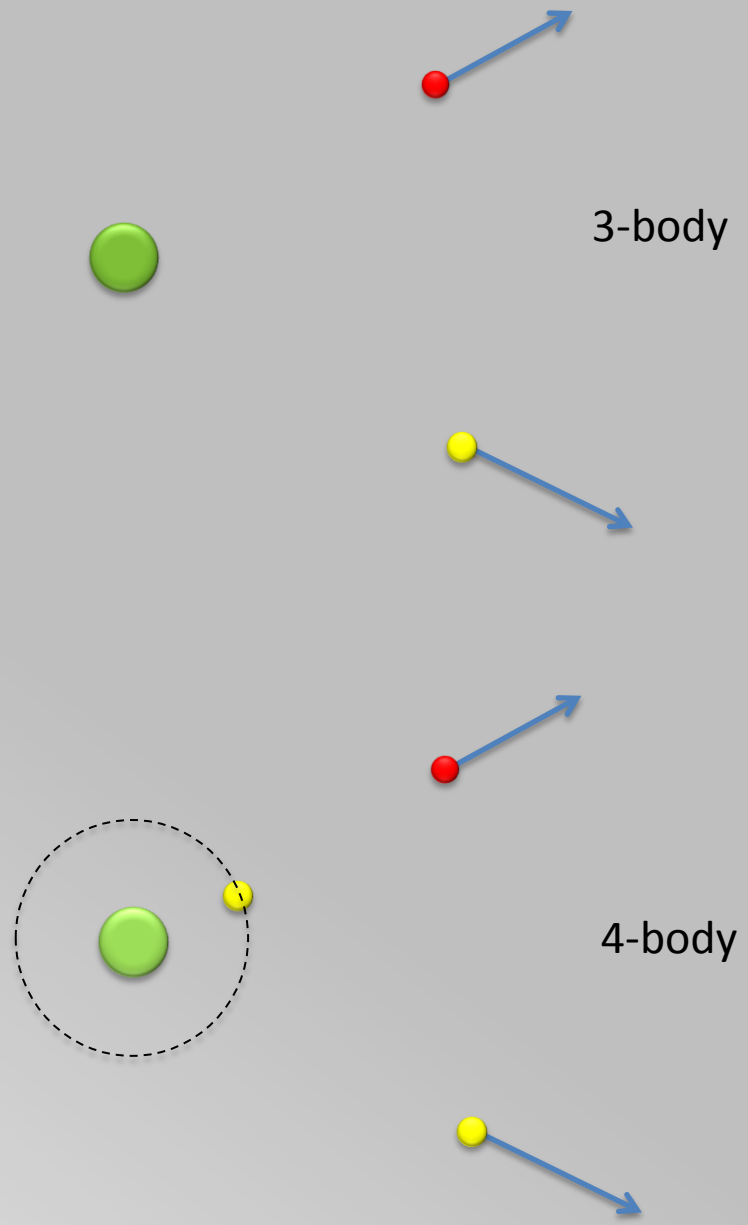
3-body

none

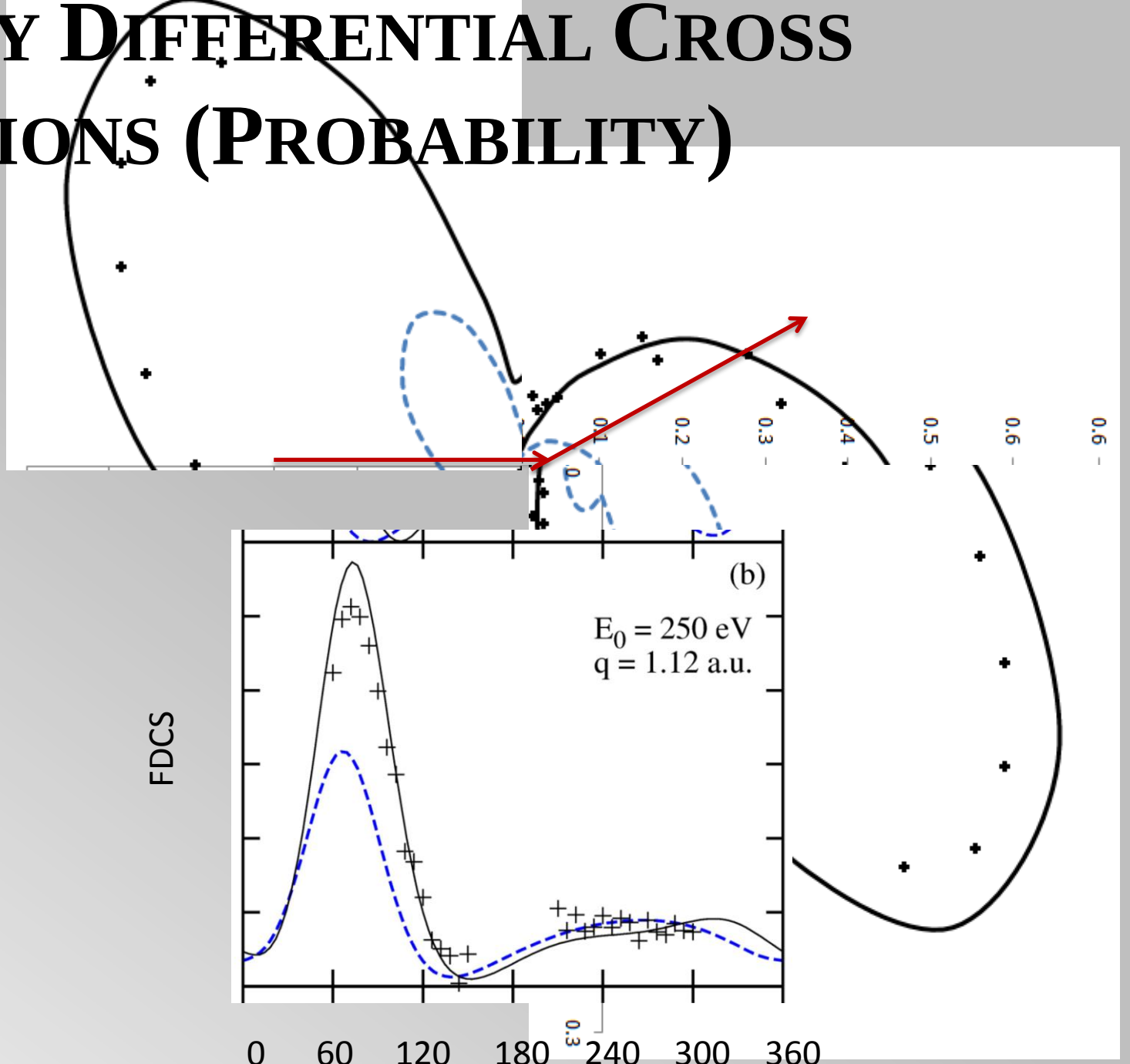
4-body

He^+ wf

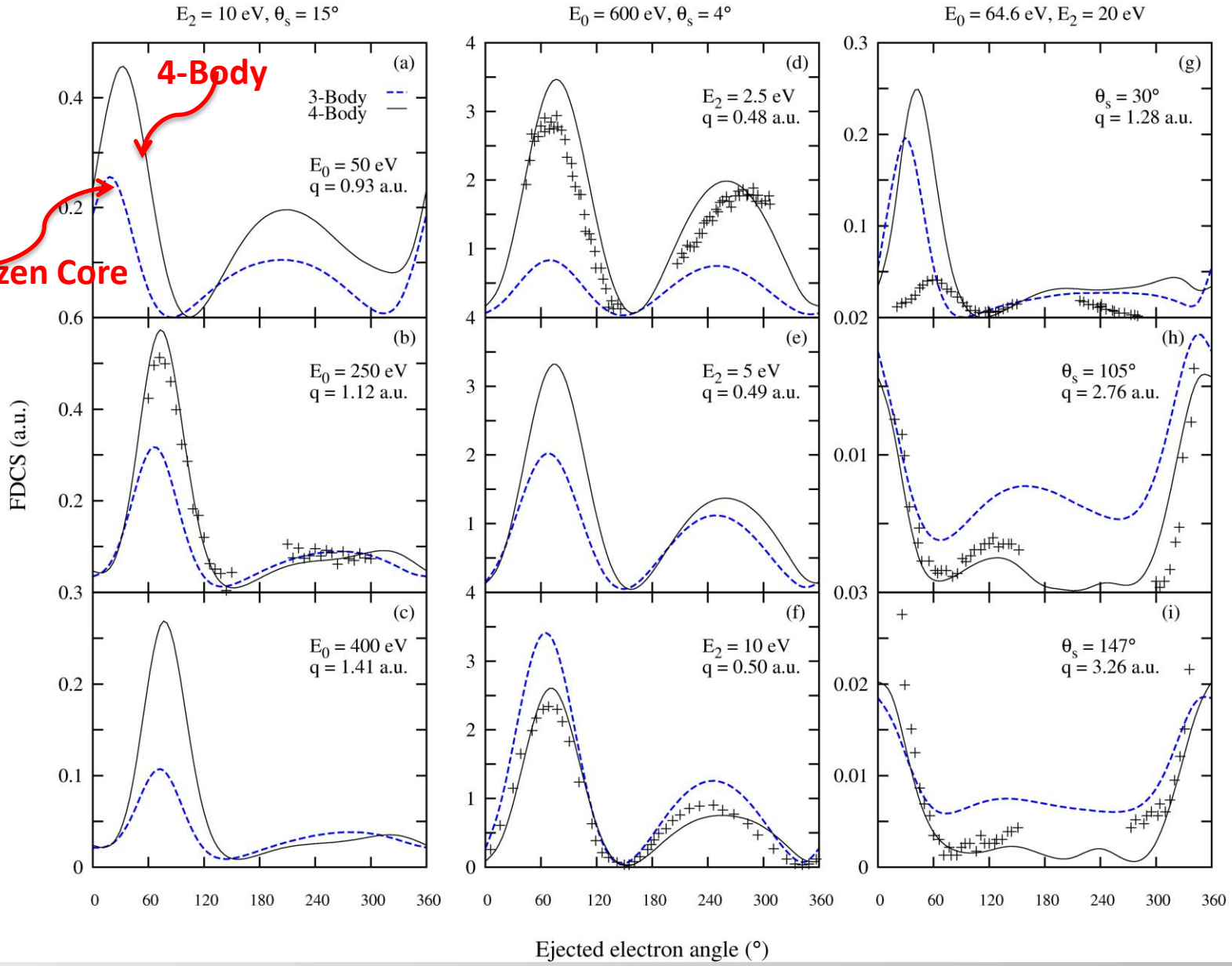
4. Final state free electrons move in different potentials



Fully Differential Cross Sections (Probability)



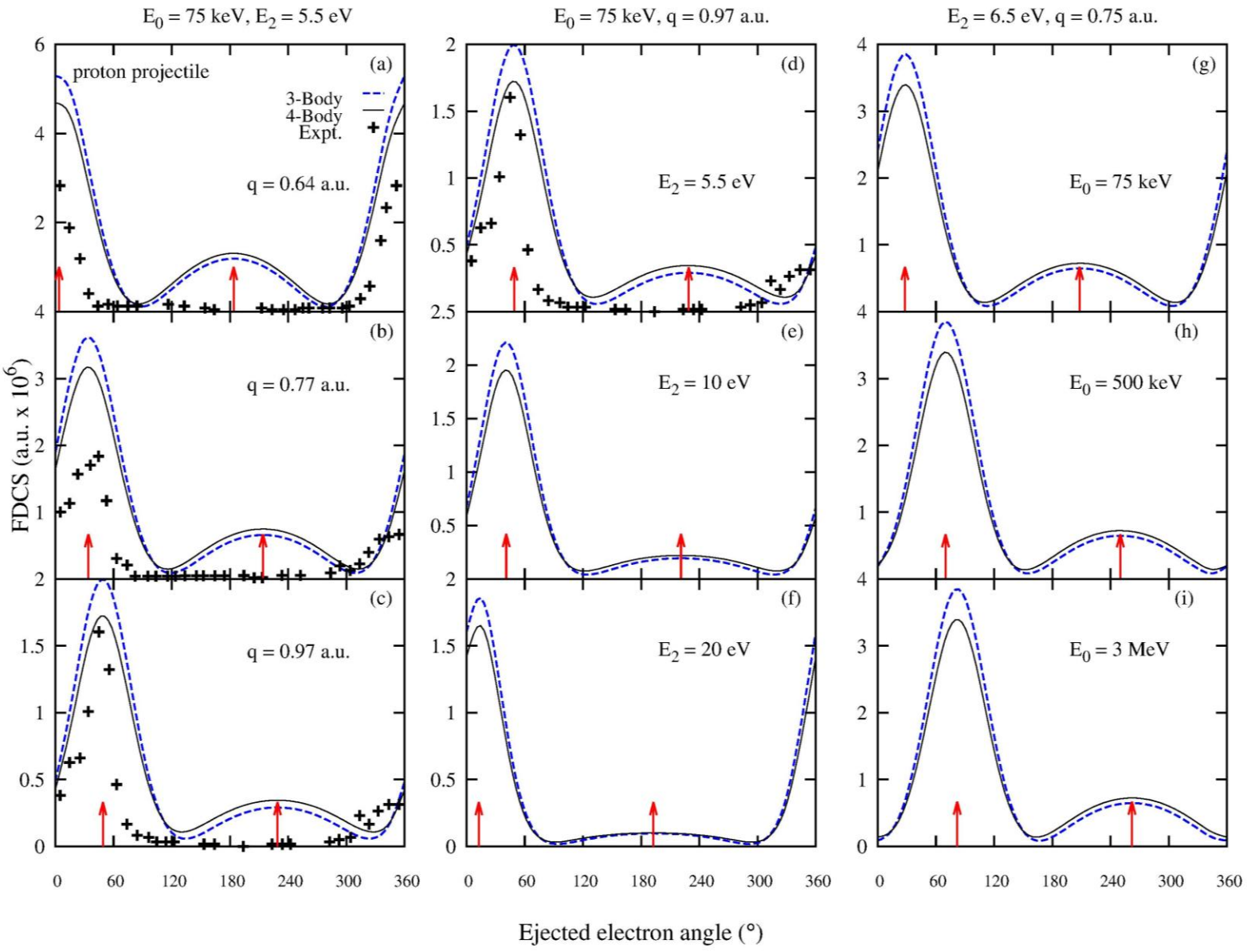
Electron Projectile



Expt: Schlemmer P, Srivastava M K, R¨osel T and Ehrhardt H 1991 J. Phys. B: At. Mol. Opt. Phys. 24 2719
Jung K, Muller-Fiedler R, Schlemmer P, Ehrhardt H and Klar H 1985 J. Phys. B: At. Mol. Phys. 18 2955
Bray I, Fursa D V, R¨oder J and Ehrhardt H 1997 J. Phys. B: At. Mol. Opt. Phys. 30 L101

Published in
J. Phys. B 46, 145202 (2013).

PROTON PROJECTILE



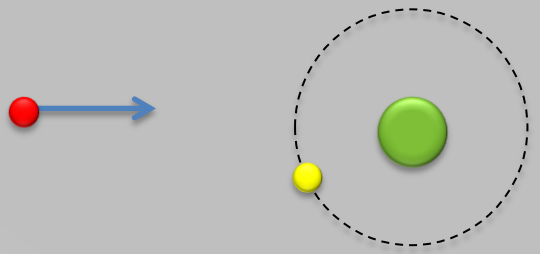
PUBLISHED IN:
J. PHYS. B 48, 115203 (2015).

Expt from: Maydanyuk et al., Phys. Rev. Lett. **94** 243201 (2005)

What part of frozen core approximation causes differences in FDCS?

1. Initial state helium wave function

- Use 4-body model
- Replace 2 electron helium wave function with 2 independent 1-electron wave functions



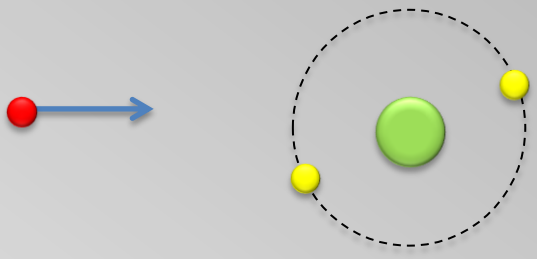
3-body

3-body

1 e^- wf

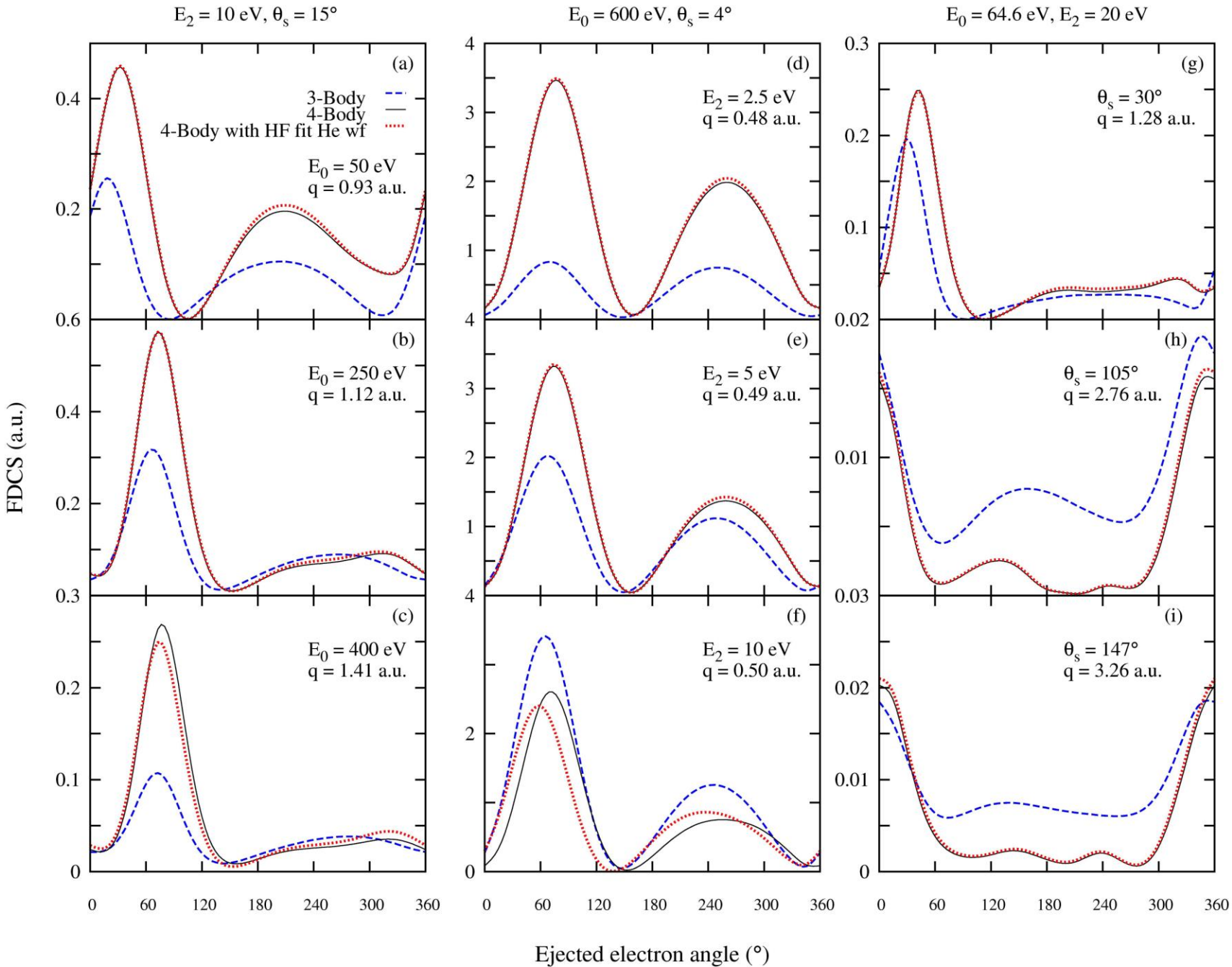
4-body

2 e^- wf with correlation



4-body

ELECTRON PROJECTILE

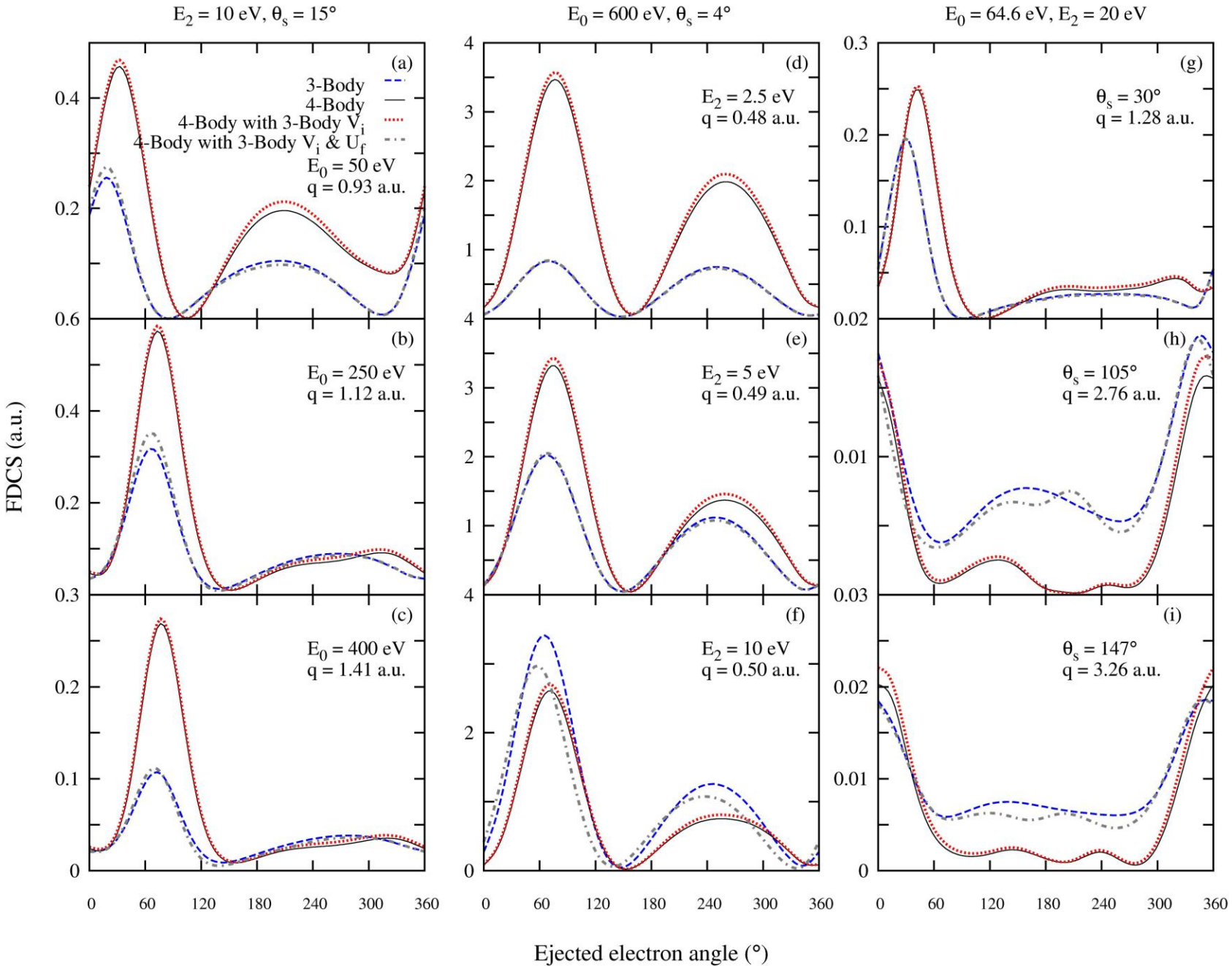


- Initial state helium wave function not source of discrepancies
- Repeat testing procedure for other possible sources

- ……..

- The answer is …
- The treatment of the ionized electron combined with the initial state perturbation is the source
- True for electrons and heavy ions

PERTURBATION AND FINAL STATE POTENTIAL



Frozen Core Approximation Conclusions

- Differences between 3-body and 4-body model caused primarily by treatment of ionized electron
- Some "additive" effect of final state potential and perturbation potential

- More info: J. Phys. B 48, 115203 (2015).
  J. Phys. B 46, 145202 (2013).

Atomic Collisions

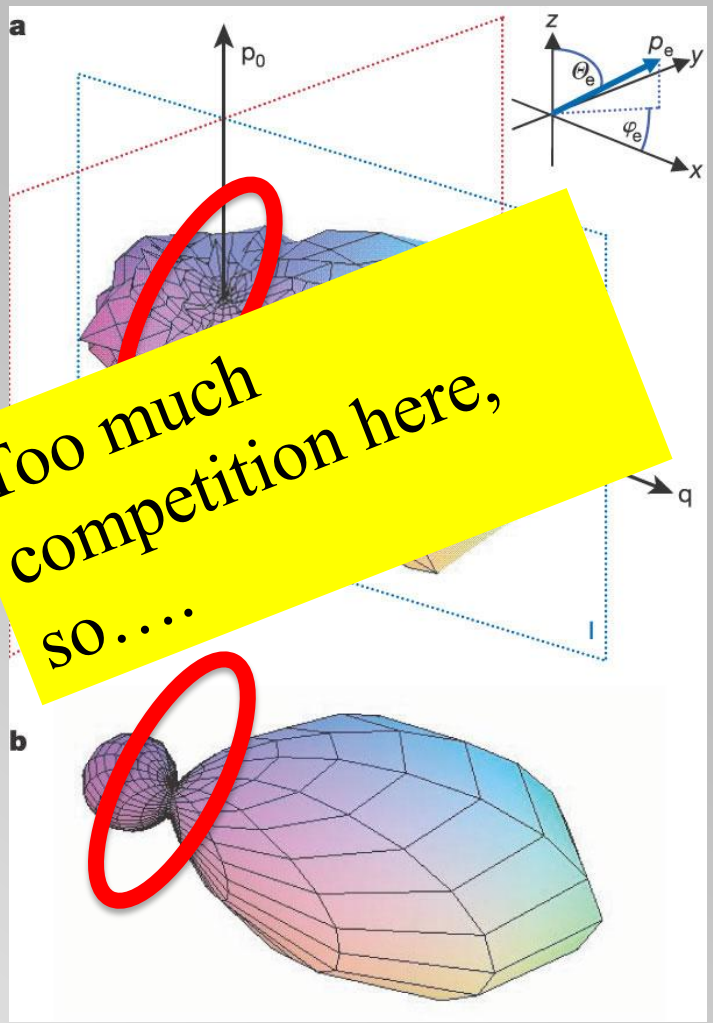
- Problems of Interest - Ionization
  - Frozen Core Approximation
  - Out-of-Plane Collisions

Classical Picture

- Plane of table is called scattering plane
- Defined by initial and final momentum vectors of projectile

- Typically ionized electron stays in the scattering plane
- Can be found outside of scattering plane (off the table)
- Theory currently can’t explain experimental results

3D FDCS for Ionization

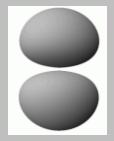


C^{6+} + He ionization

M. Schulz, et al., *Nature* **422**, 48 (2003).

3D FDCS for Excitation-Ionization

- True 4-body process
- Possible orientation effects of He^+ ion

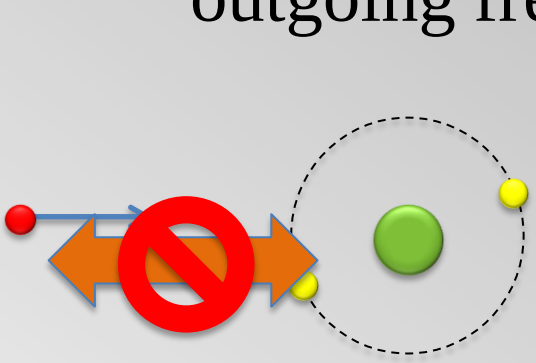


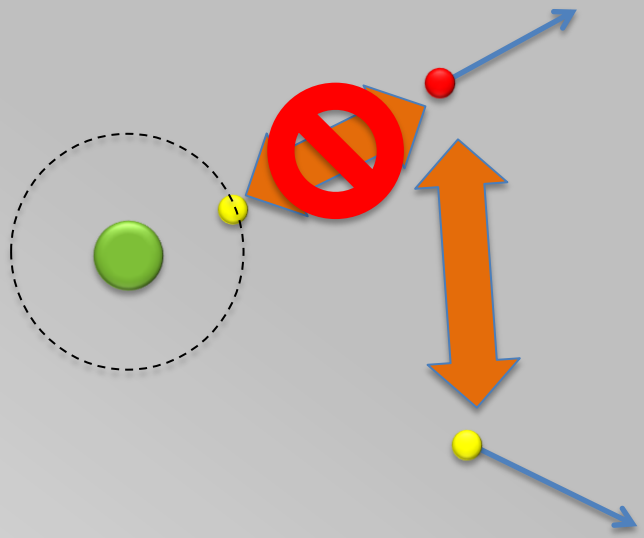
Excitation-Ionization of Helium

Oleg Zatsarinny and Klaus Bartschat, *J. Phys. B: At. Mol. Opt. Phys.* **47,** 06100 (2014)). See http://iopscience.iop.org/0953-4075/47/6/061001/ for video

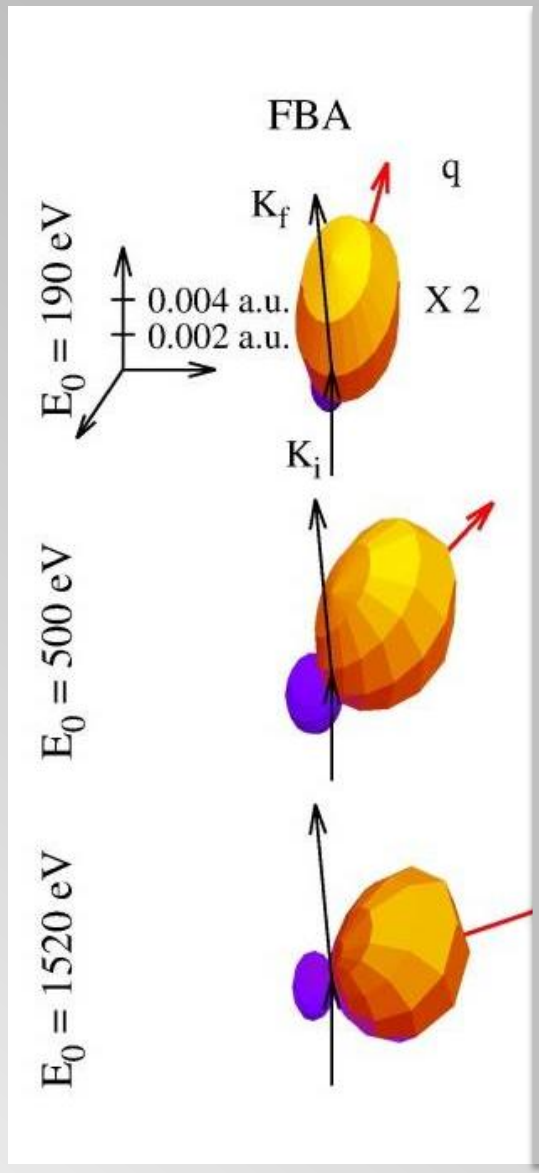
Models

- FBA
  - Projectile plane wave (no interaction with target)
- 4DW – No PCI
  - Projectile distorted wave (interaction with target)
- 4DW
  - All 2-particle interactions, including between outgoing free particles





3D FDCS



3D Excitation-Ionization Conclusions (Preliminary)

- Projectile interactions with target enhance backward emission of electron
- Interaction between outgoing particles further enhances backward emission of electron
- Why? Not sure yet…..

STUDENTS

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Frozen Core
Approximation

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3D Excitation-
Ionization

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4-Body Ionization

Annabelle Shaffer
Computational
Neuroscience

Thank You!