Capture of Slow Antiprotons by Atoms, Molecules, and Ions

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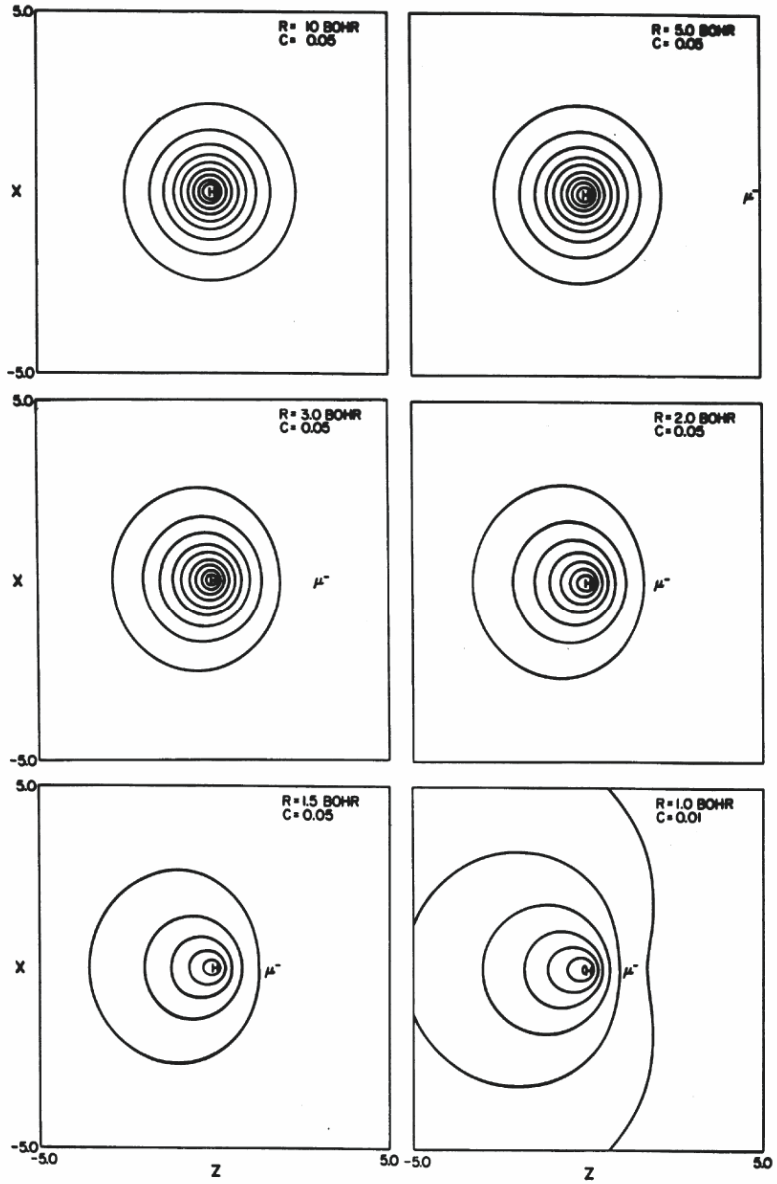
Workshop on Physics with Ultra-Slow Antiproton Beams
RIKEN, March 14–16, 2005

What do we think we know and what can be verified using the new capability with slow antiproton beams?

Recent review (mainly theoretical): J.S. Cohen, *Rep. Prog. Phys.* **67**, 1769-1819 (2004).

Adiabatic μ^- (or $\bar{p}$) + H

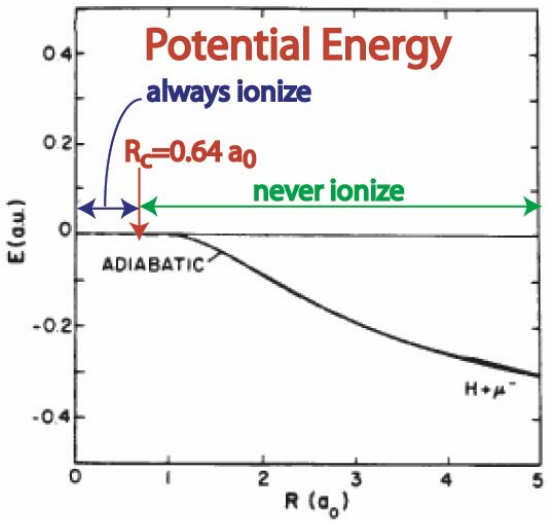


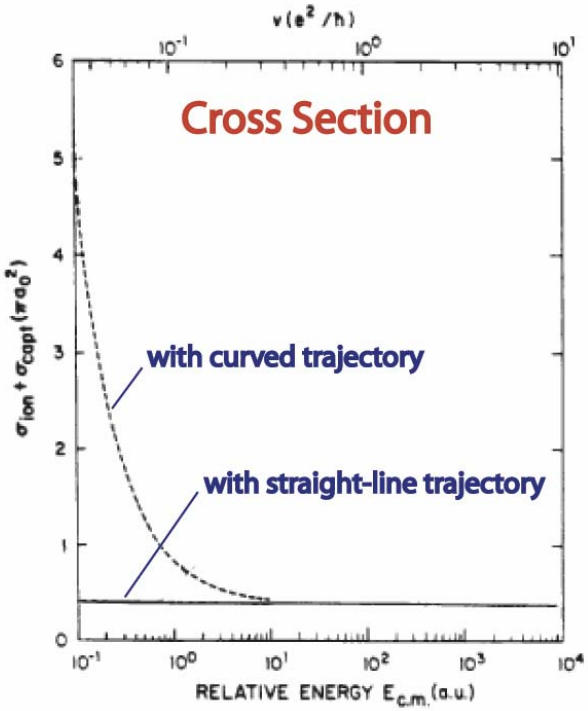
"Adiabatic ionization" occurs at $R < R_c \approx 0.64\ a_o$

[Wightman, 1950; Fermi&Teller, 1947]

ADIABATIC IONIZATION

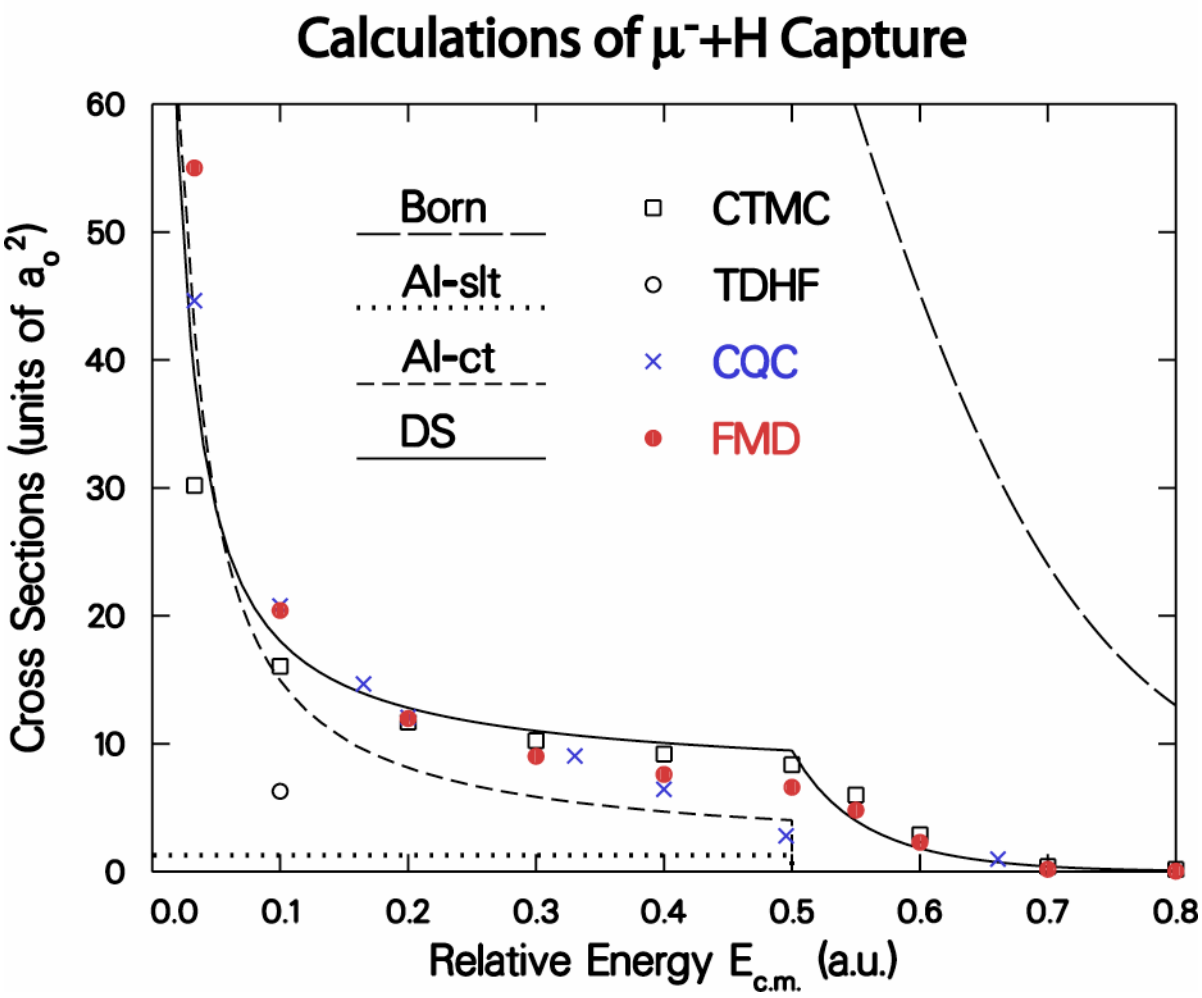
$x^- + H$ $(x^- = \mu^-, \pi^-, \bar{p})$

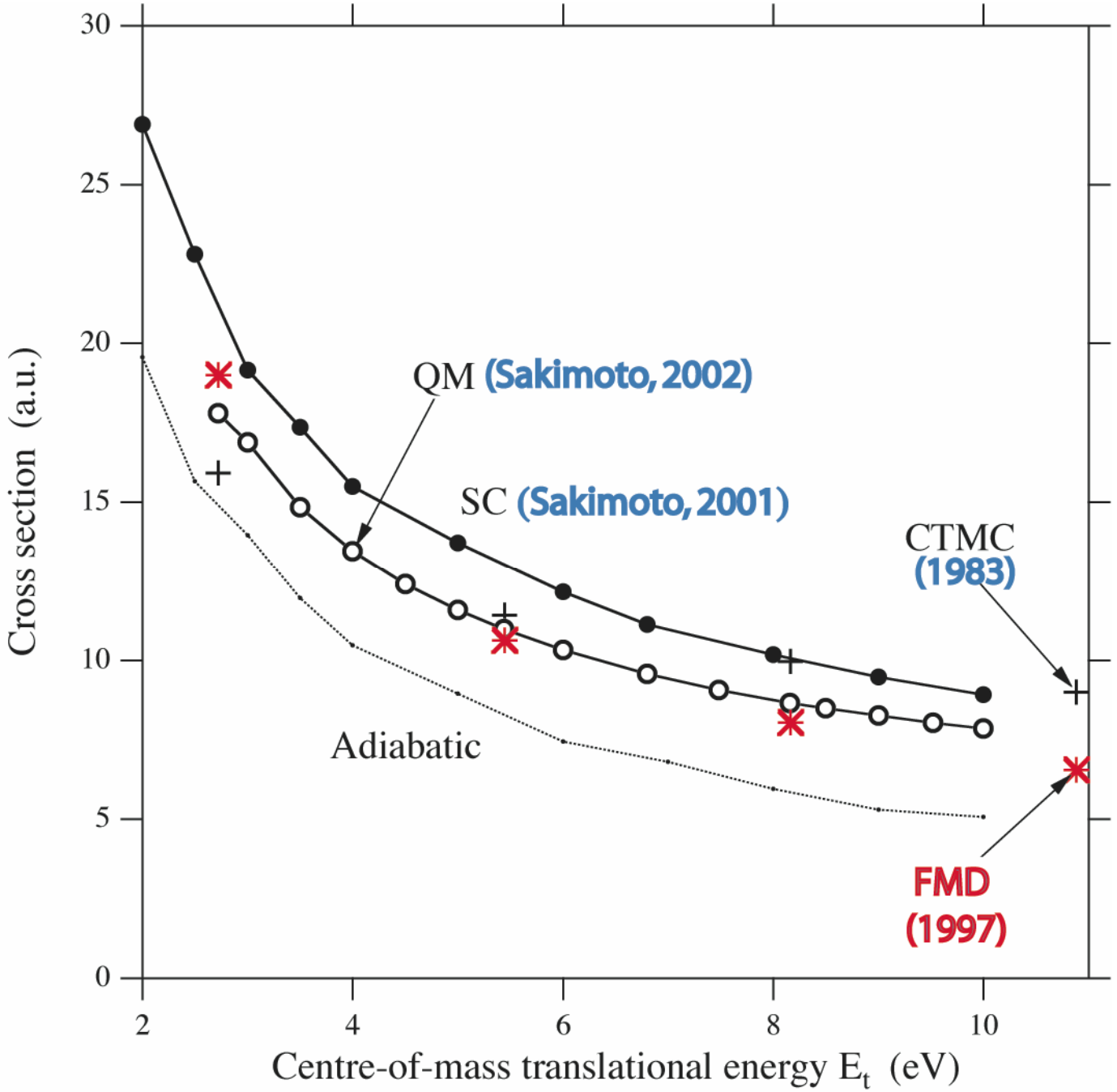


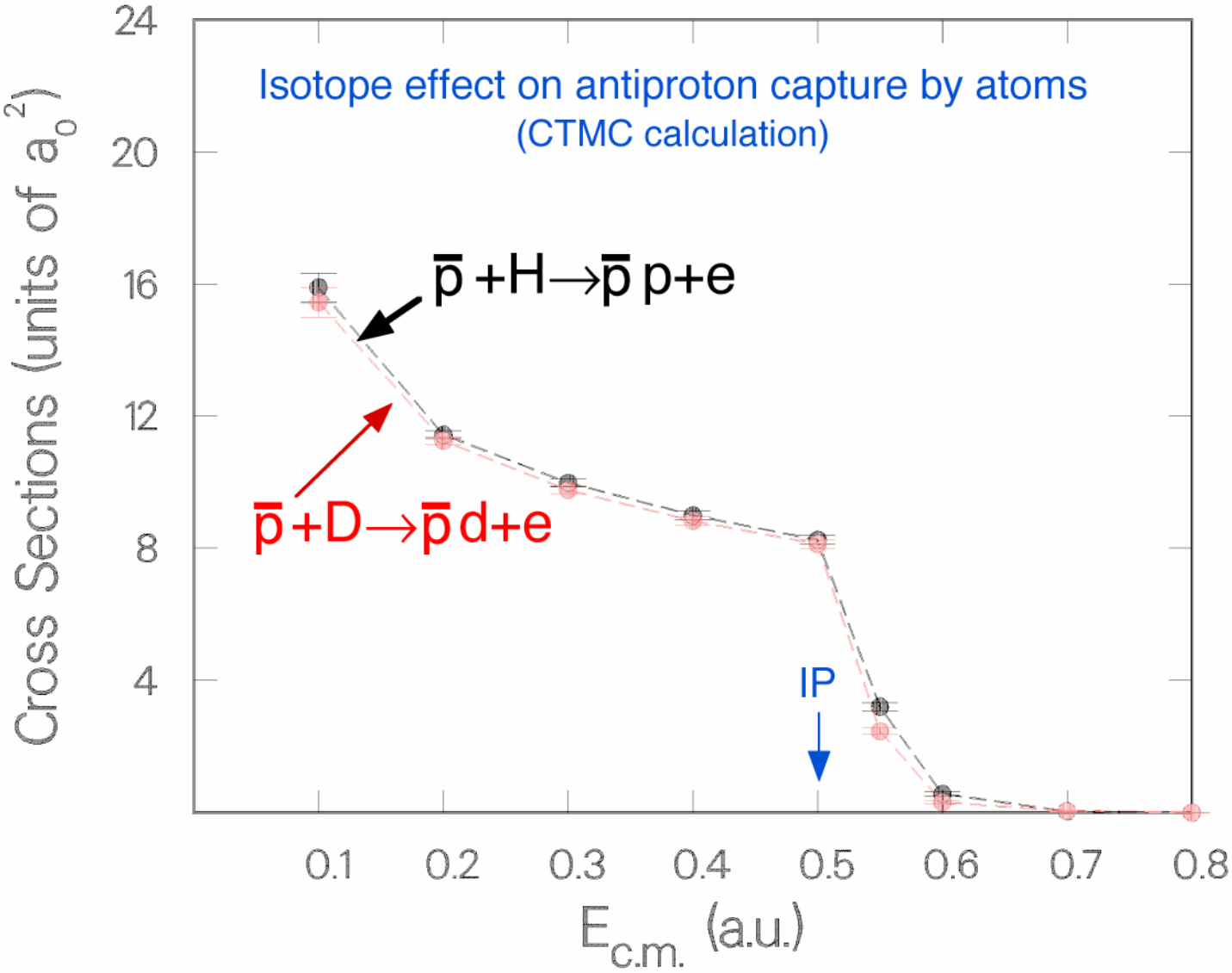


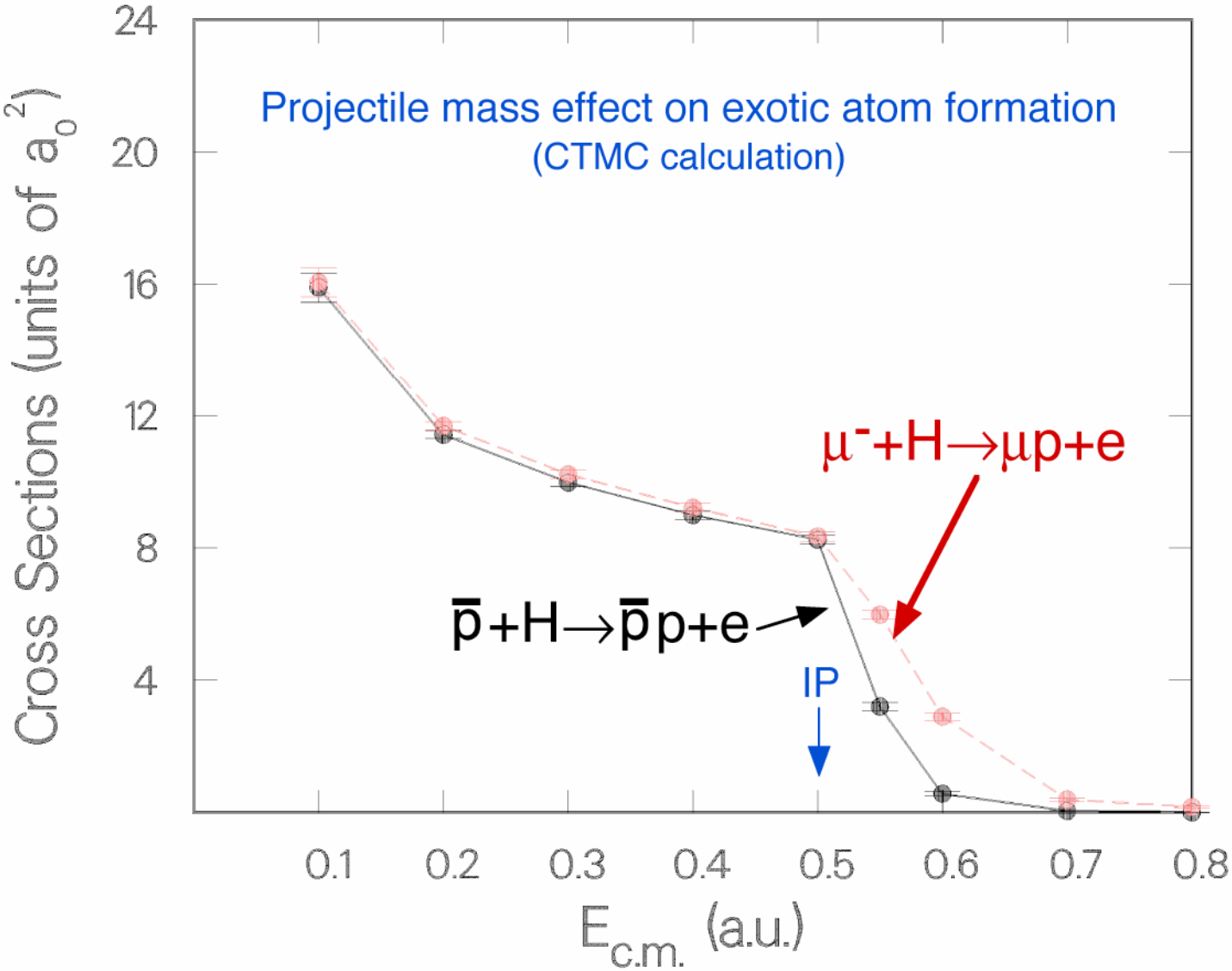
Theoretical methods for X^- capture by the H *atom*

1. Adiabatic ionization (AI)
   [Wightman(1950)]
2. Born / Coulomb-Born (BA, DWA)
   [de Borde(1954) ... Korenman & Rogovaya(1980)]
3. Diabatic states (DS)
   [Cohen, Martin & Wadt(1981)]
4. Classical-trajectory Monte Carlo (CTMC)
   [Cohen(1983)]
5. Time-dependent Hartree-Fock (TDHF) with μ wave packet
   [Garcia, Kwong & Cohen(1987)]
6. Classical-quantal coupling (CQC)
   [Kwong, Garcia & Cohen(1989)]
7. Close coupling (CC)
   [Boukour(1996)]
8. Fermion molecular dynamics (FMD)
   [Cohen(1997, 1998)]
9. Perturbed stationary states (PSS)
   [Ohtsuki(1999)]
10. Time-dependent semiclassical(trajectory) Schrödinger eq. (SC)
    [Sakimoto(2001)]
11. Time-dependent wavepacket Schrödinger equation (QM)
    [Sakimoto(2002)]


Calculations of μ⁻+H Capture
Cross Sections (units of a_o^2)
Relative Energy $E_{c.m.}$ (a.u.)
Born
AI-slt
AI-ct
DS
CTMC
TDHF
CQC
FMD
0
10
20
30
40
50
60
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8


30
25
20
15
10
5
0
2
4
6
8
10
Cross section (a.u.)
Centre-of-mass translational energy E_t (eV)
QM (Sakimoto, 2002)
SC (Sakimoto, 2001)
CTMC
(1983)
Adiabatic
FMD
(1997)


Isotope effect on antiproton capture by atoms
(CTMC calculation)
$\bar{p}$ +H→$\bar{p}$ p+e
$\bar{p}$ +D→$\bar{p}$ d+e
IP
Cross Sections (units of a_o^2)
24
20
16
12
8
4
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
$E_{c.m.}$ (a.u.)


Projectile mass effect on exotic atom formation
(CTMC calculation)
Cross Sections (units of a_o^2)
24
20
16
12
8
4
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
$E_{c.m.}$ (a.u.)
$\mu^-+H\rightarrow\mu p+e$
$\bar{p}+H\rightarrow\bar{p}p+e$
IP

The Quasiclassical Method

The Fermion Molecular Dynamics (FMD) method is an extension of the Classical-Trajectory Monte Carlo (CTMC) method to multi-electron atoms and molecules, obtained by introducing pseudo-potentials to represent quantum-mechanical effects.

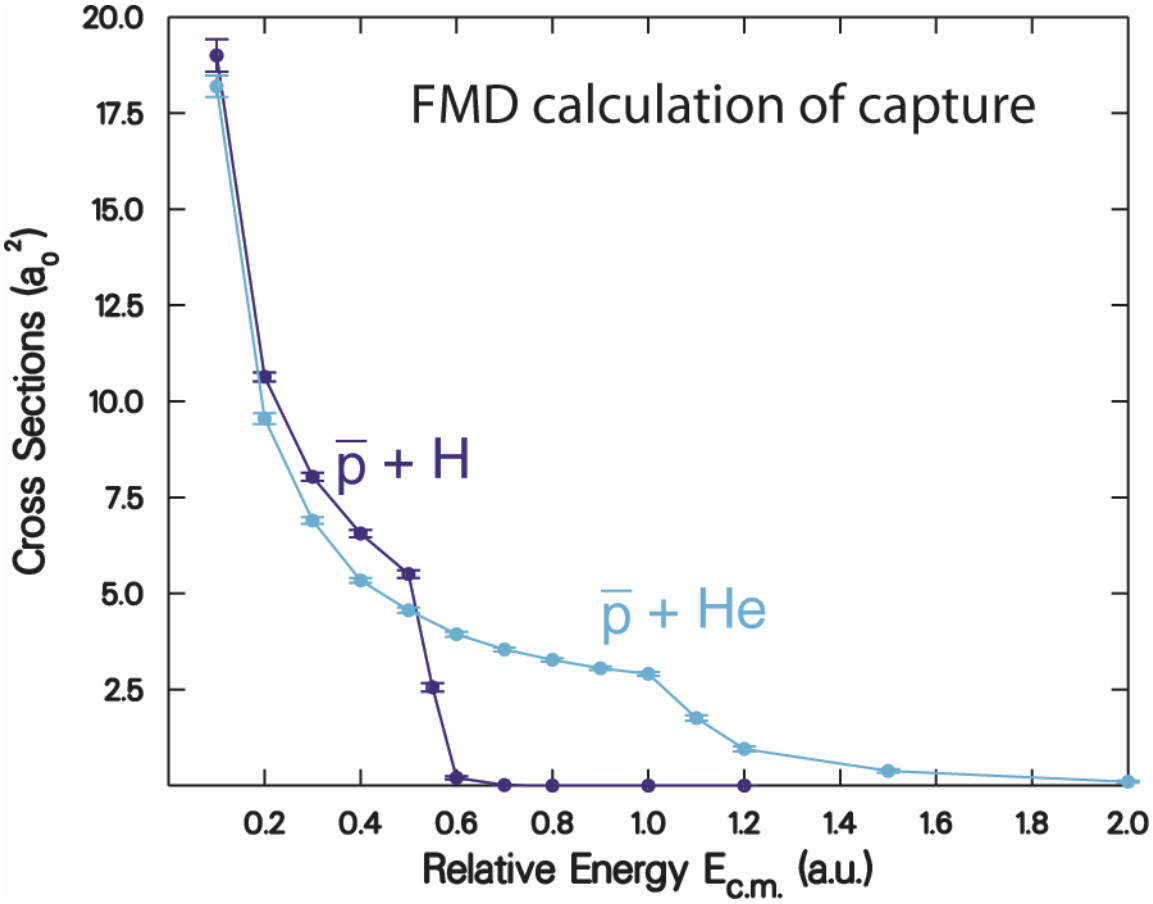
Advantages for capture of heavy ($m \gg m_e$) negative particles:

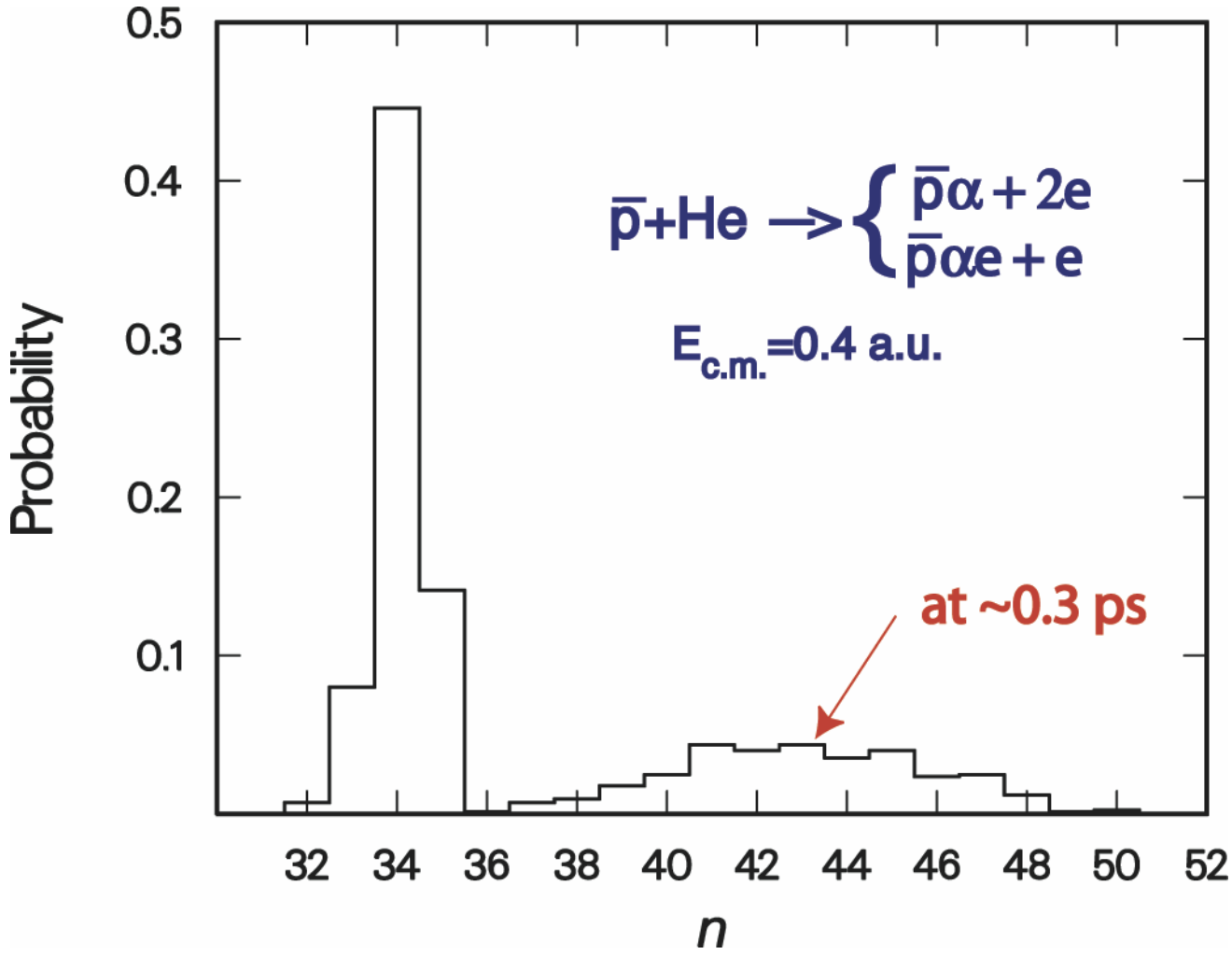
- The classical (Hamilton) equations of motion are easier to solve than the Schrödinger equation.
- Full dynamics is done for all particles. Thus correlation is fully treated and all rearrangement channels (including breakup) are treated on equal footing.
- The electronic continuum occurs naturally.
- The large number of intermediate and final states presents no difficulty. Capture is into high n, l orbitals, so the correspondence principle applies.

Possible weaknesses:

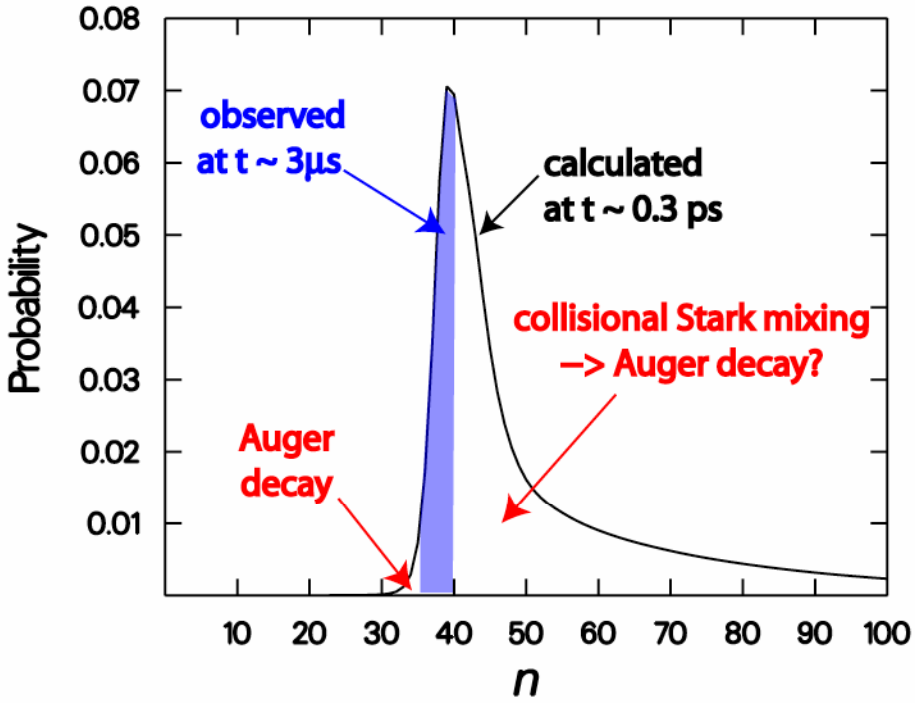
- Correlation may be too strong.
- May not be adequate when the molecular vibrational–rotational spacings are large (as in H_2).
- Not valid for light reactants like electrons and positrons.

Where corroboration is available, the FMD method seems to be rather accurate, but, at the very least, it is useful to obtain an indication of important features, so requirements for experiments and future quantum-mechanical methods can be gauged.


FMD calculation of capture
Cross Sections (a_0^2)
Relative Energy $E_{c.m.}$ (a.u.)
$\bar{p}$ + H
$\bar{p}$ + He
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0


0.5
0.4
0.3
0.2
0.1
Probability
$\bar{p}$+He → { $\bar{p}\alpha + 2e$; $\bar{p}\alpha e + e$
$E_{c.m.}$=0.4 a.u.
at ~0.3 ps
32
34
36
38
40
42
44
46
48
50
52
n

Metastable $\bar{p}\alpha e$

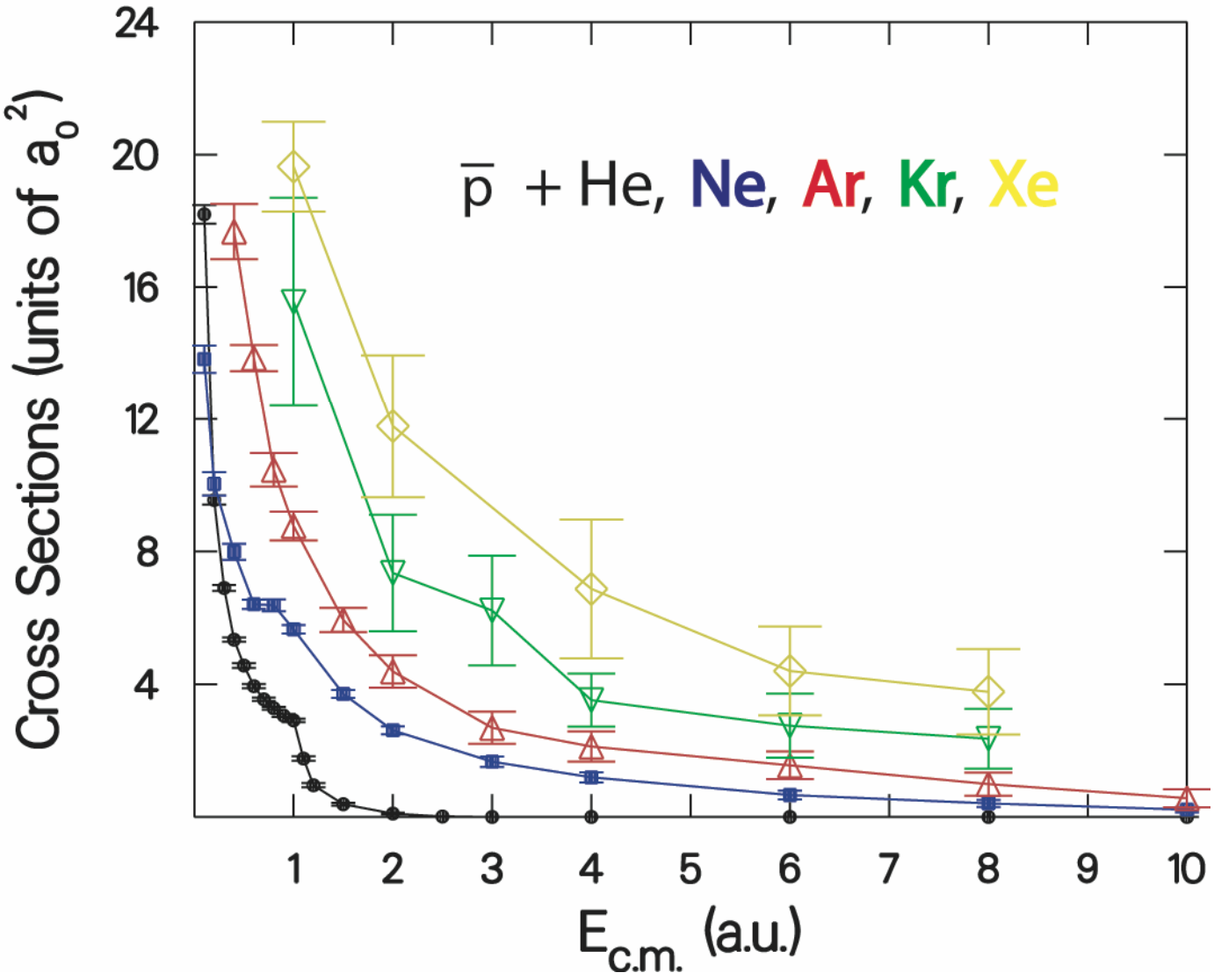


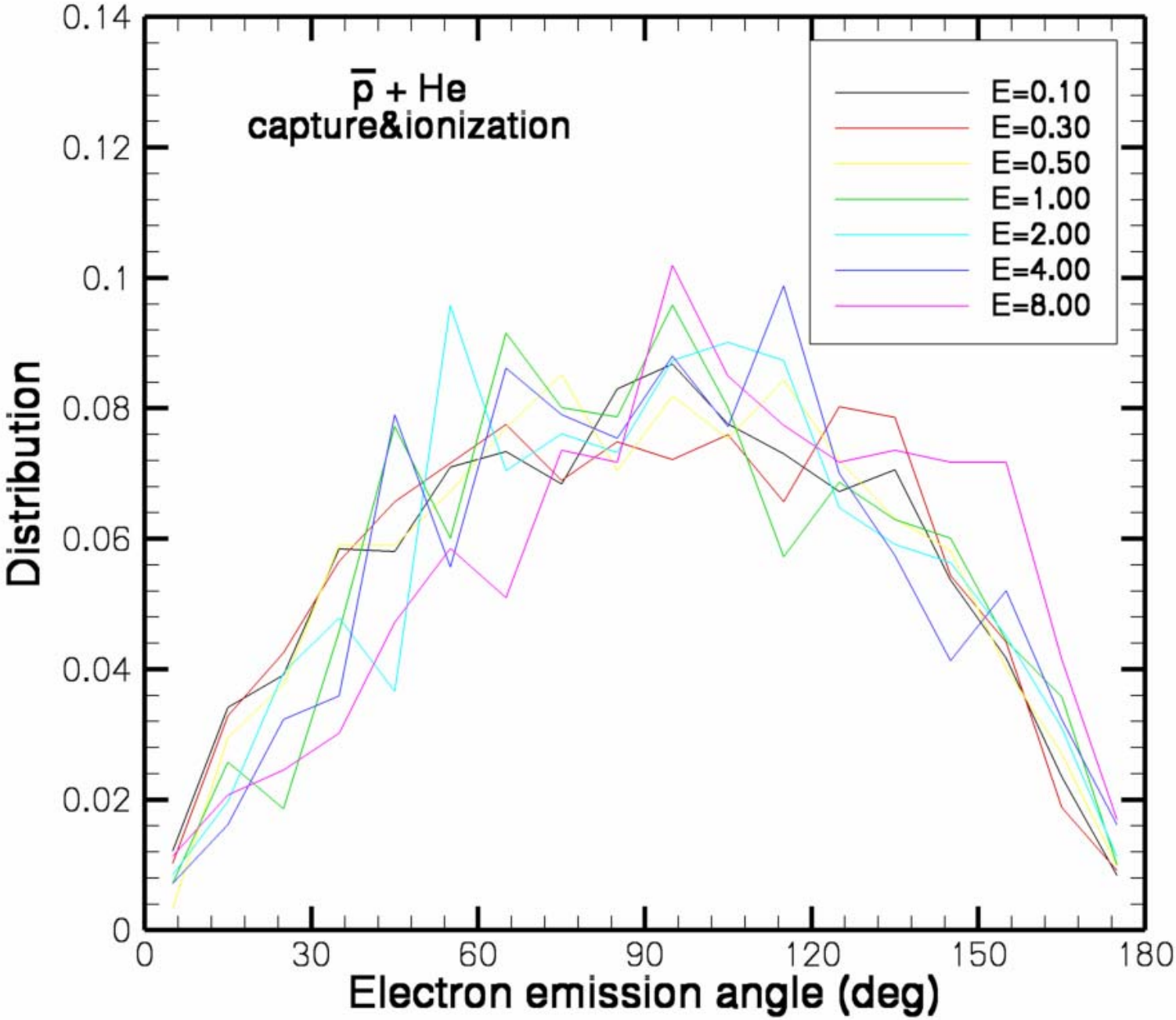
States can **Auger decay** if

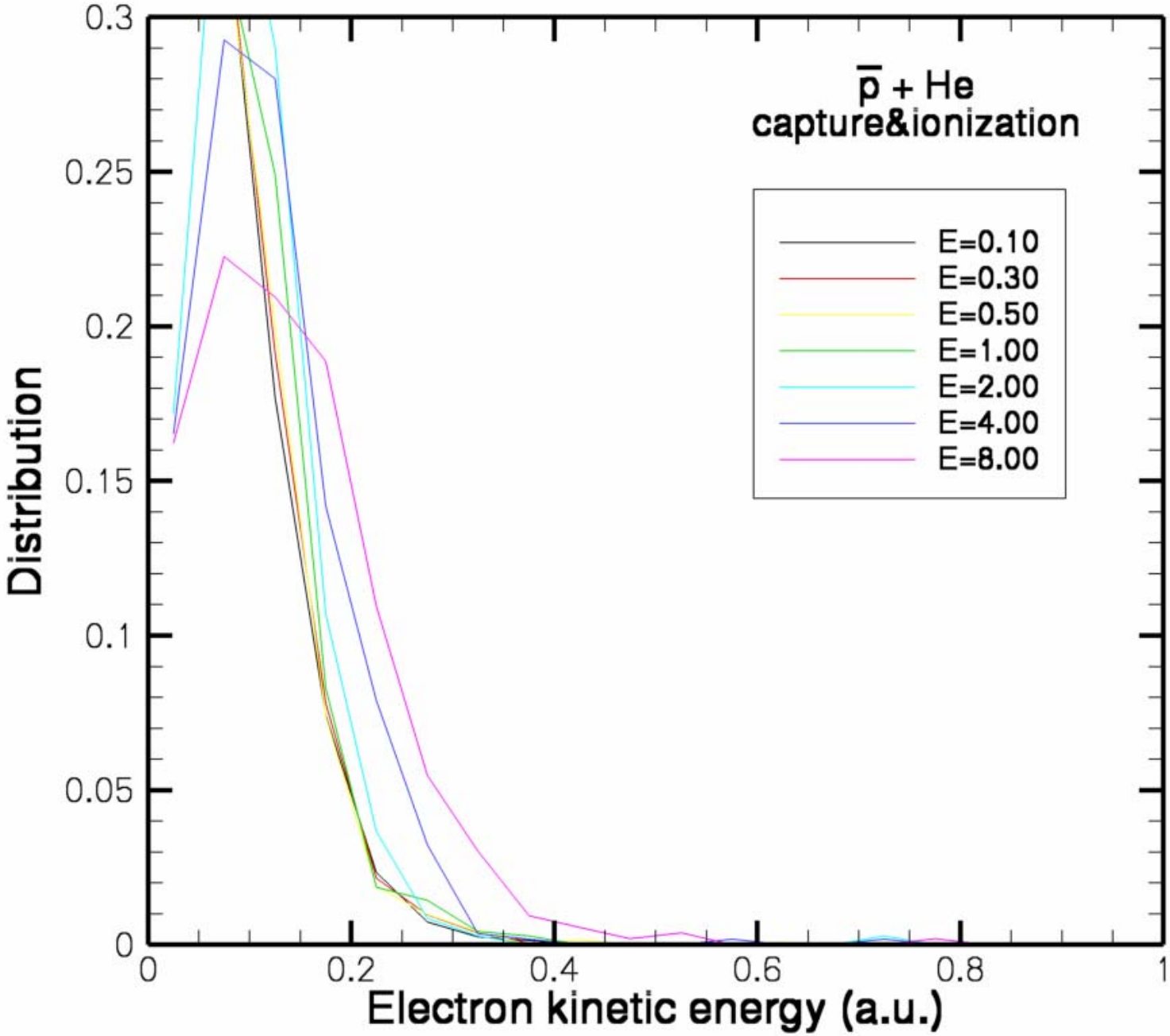
$$E_i^{(\bar{p})} - E_f^{(\bar{p})} > E_{bind}^{(e)}$$

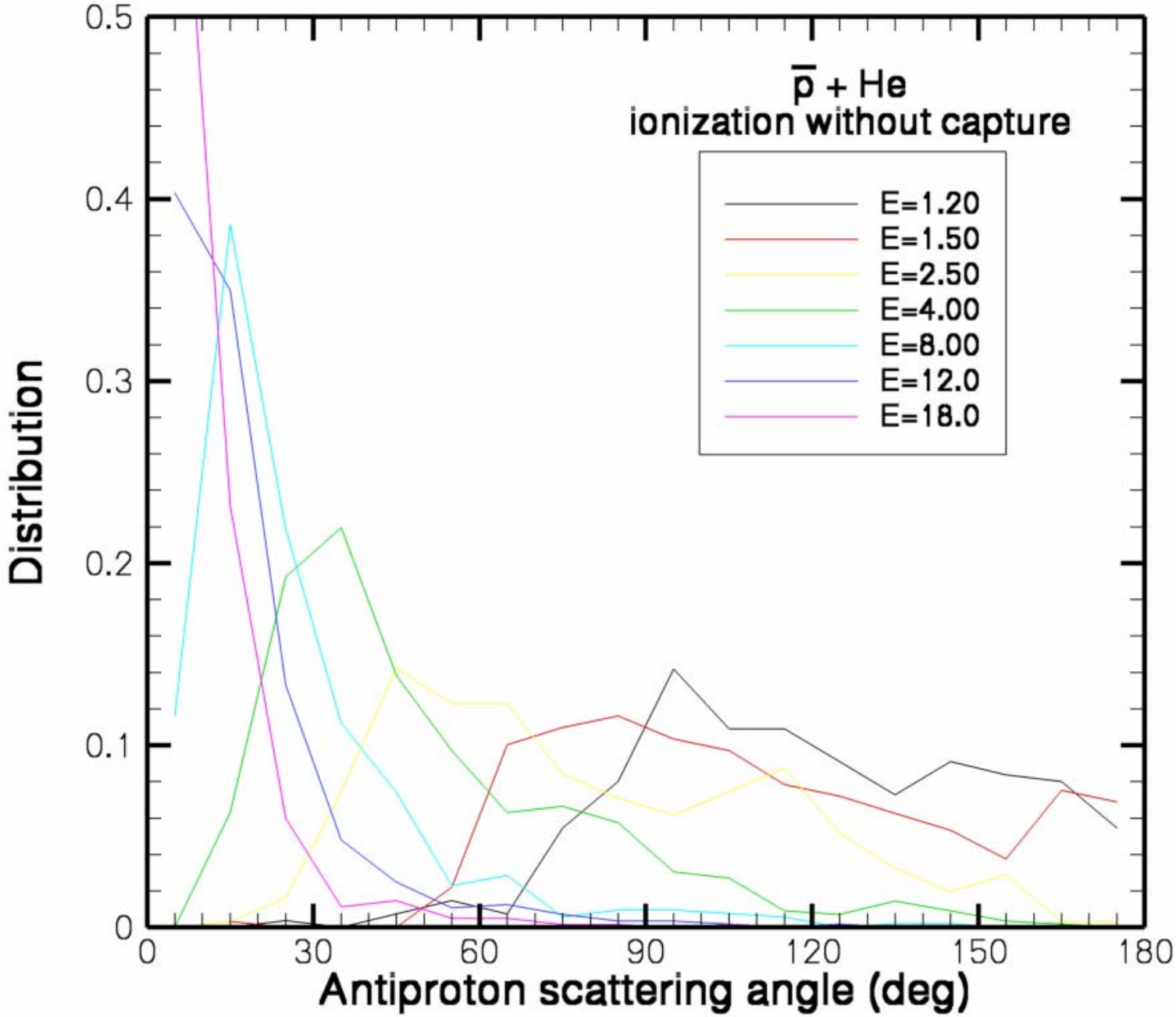
If $l=n-1$, then $\Delta n = 1$ for dipole transitions, and this condition is satisfied only for $n \lesssim 30$.

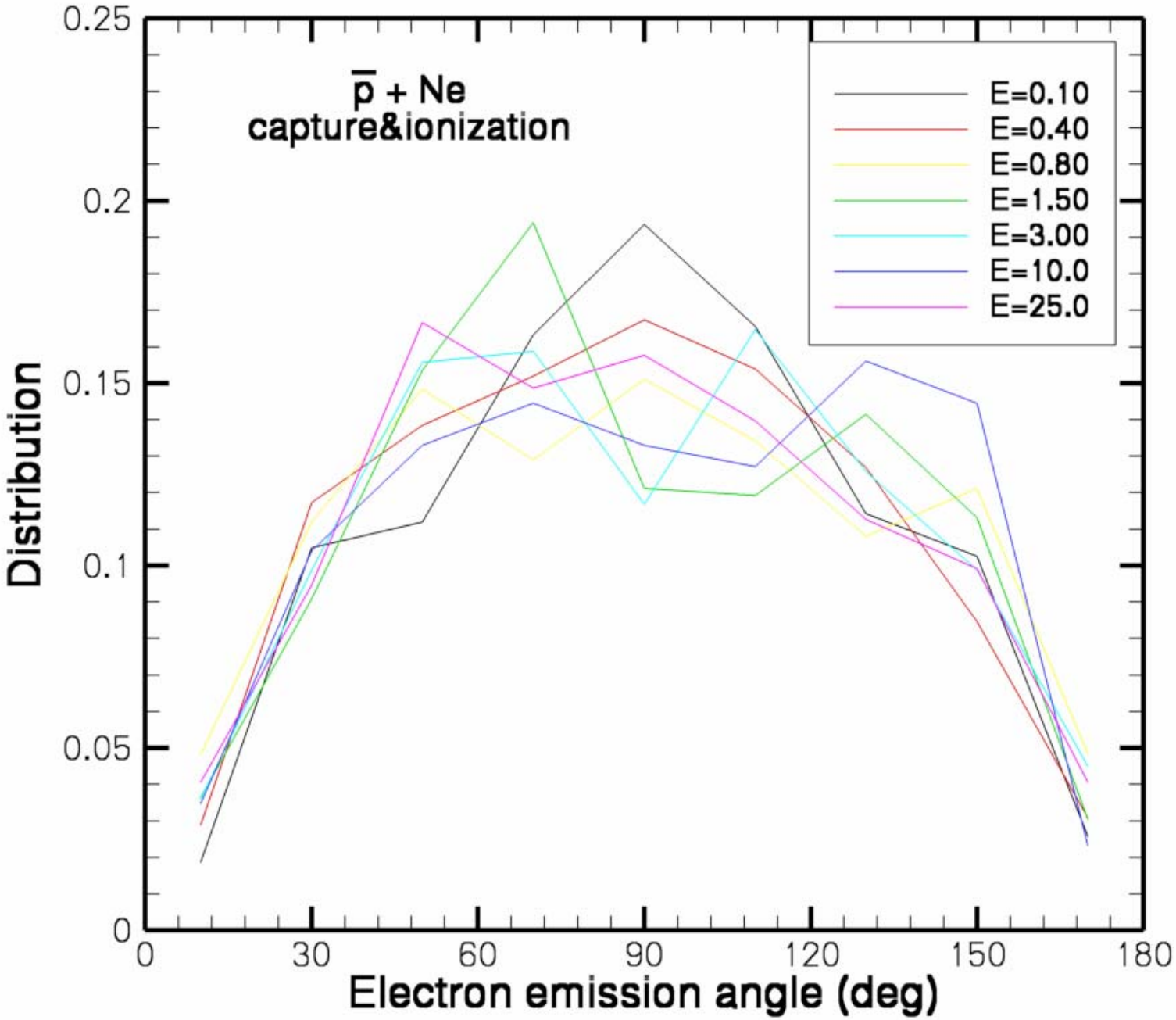
But big atoms (large n) may be collisionally **Stark mixed** so the selection rule doesn't apply.

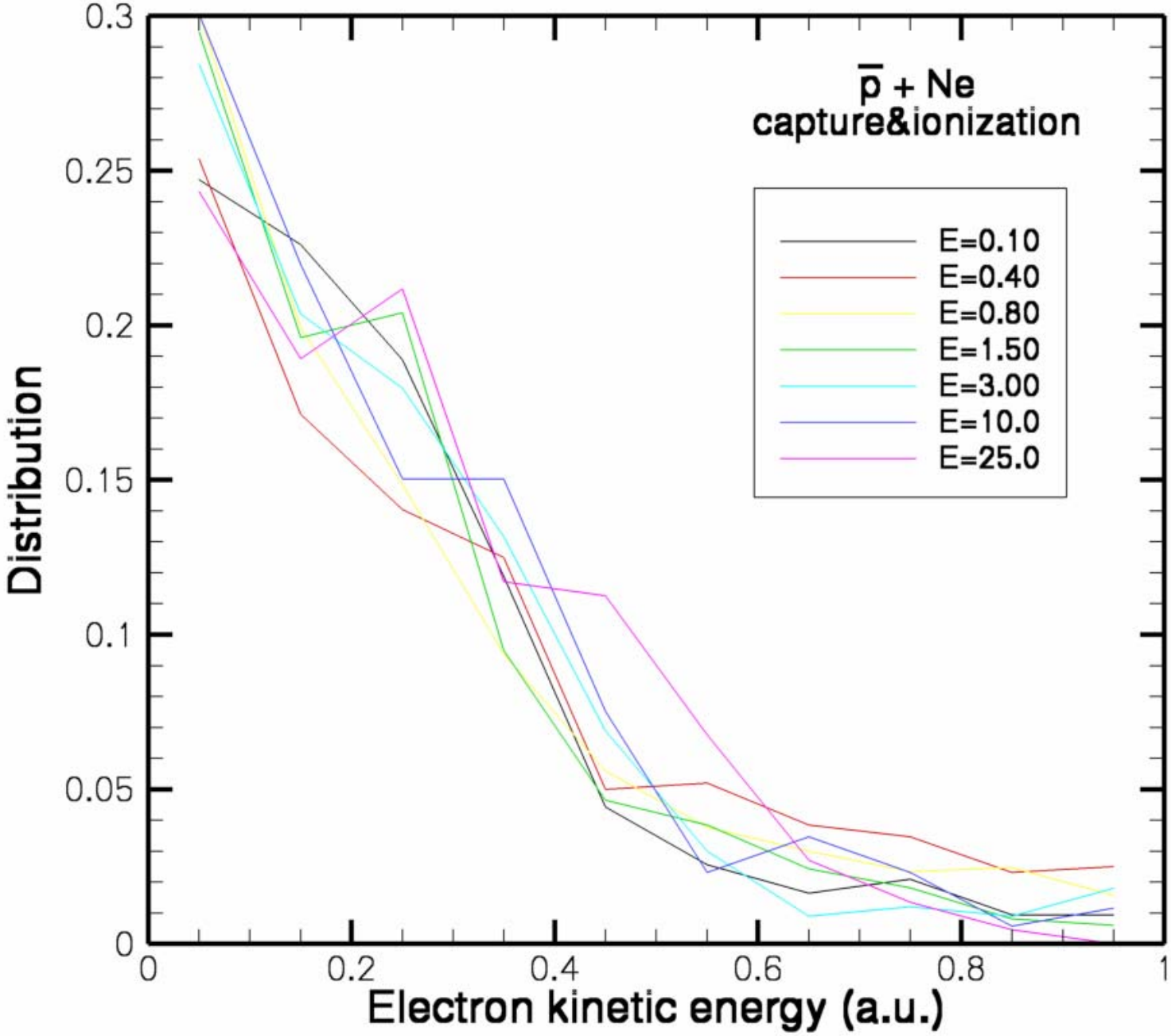

Cross Sections (units of a_0^2)
24
20
16
12
8
4
$\bar{p}$ + He, Ne, Ar, Kr, Xe
1
2
3
4
5
6
7
8
9
10
$E_{c.m.}$ (a.u.)

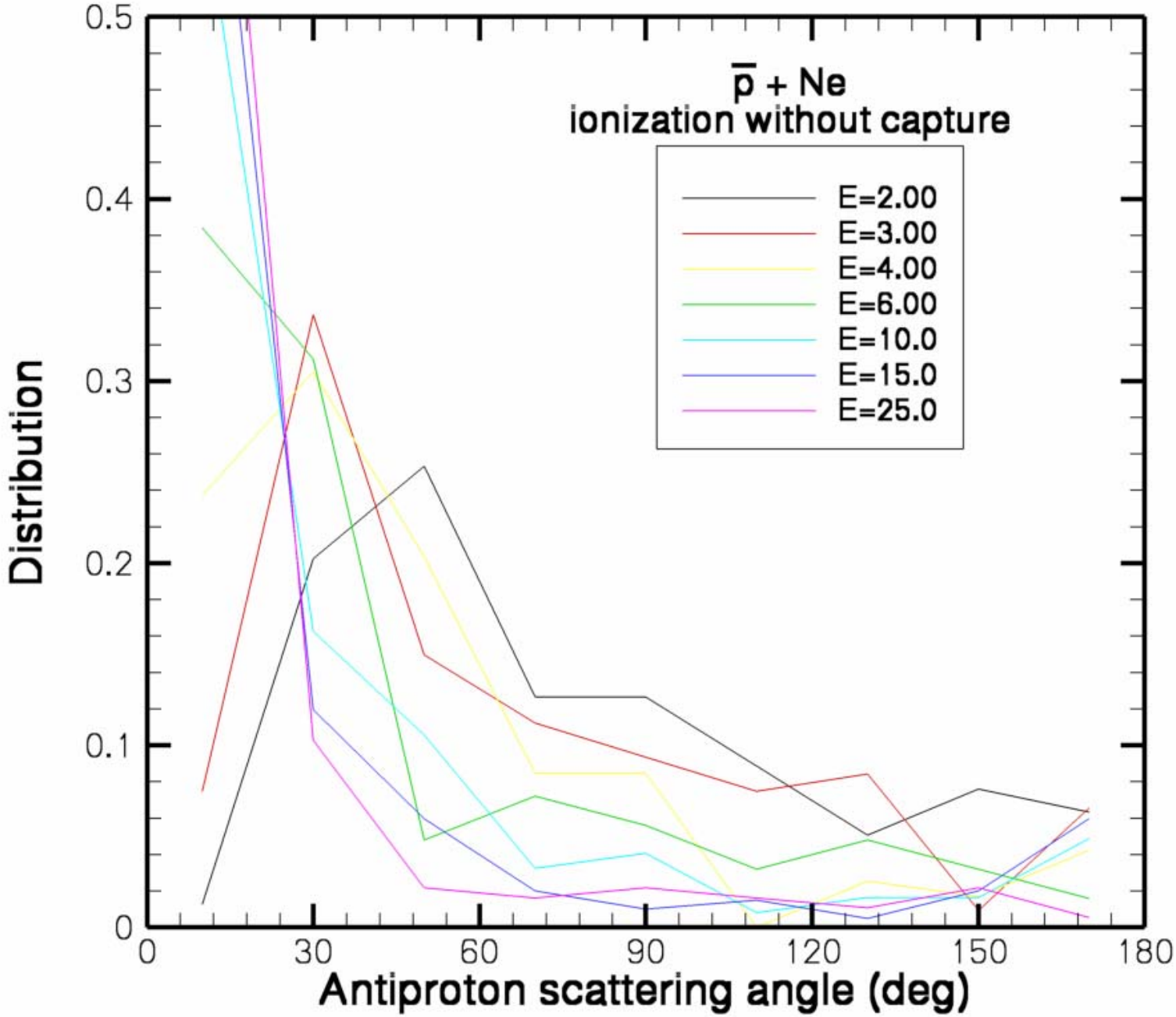

$\bar{p}$ + He
capture&ionization
E=0.10
E=0.30
E=0.50
E=1.00
E=2.00
E=4.00
E=8.00
Distribution
Electron emission angle (deg)
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0
30
60
90
120
150
180


$\bar{p}$ + He
capture&ionization
E=0.10
E=0.30
E=0.50
E=1.00
E=2.00
E=4.00
E=8.00
Distribution
Electron kinetic energy (a.u.)
0
0.05
0.1
0.15
0.2
0.25
0.3
0
0.2
0.4
0.6
0.8
1

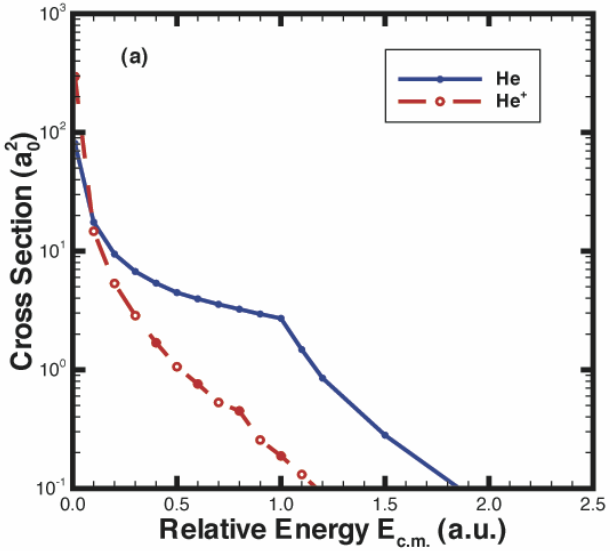

$\bar{p}$ + He
ionization without capture
E=1.20
E=1.50
E=2.50
E=4.00
E=8.00
E=12.0
E=18.0
Distribution
0
0.1
0.2
0.3
0.4
0.5
0
30
60
90
120
150
180
Antiproton scattering angle (deg)

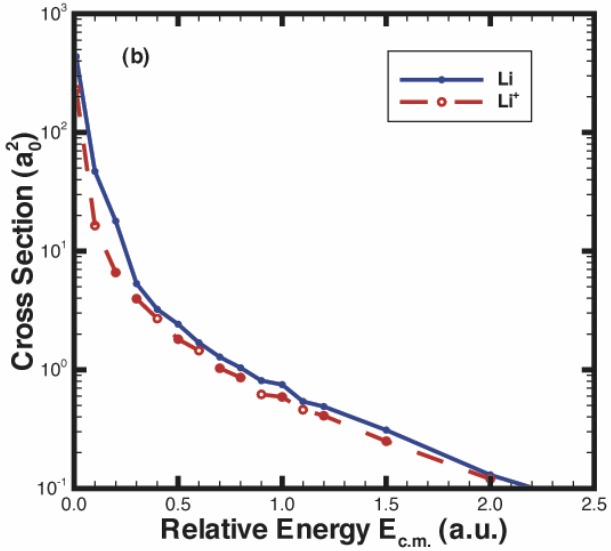

$\bar{p}$ + Ne
capture&ionization
E=0.10
E=0.40
E=0.80
E=1.50
E=3.00
E=10.0
E=25.0
Distribution
Electron emission angle (deg)
0
0.05
0.1
0.15
0.2
0.25
0
30
60
90
120
150
180

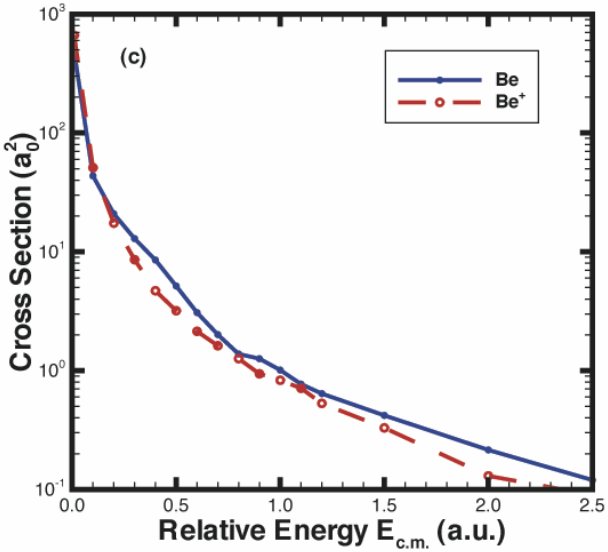

$\bar{p}$ + Ne
capture&ionization
E=0.10
E=0.40
E=0.80
E=1.50
E=3.00
E=10.0
E=25.0
Distribution
Electron kinetic energy (a.u.)
0
0.05
0.1
0.15
0.2
0.25
0.3
0
0.2
0.4
0.6
0.8
1

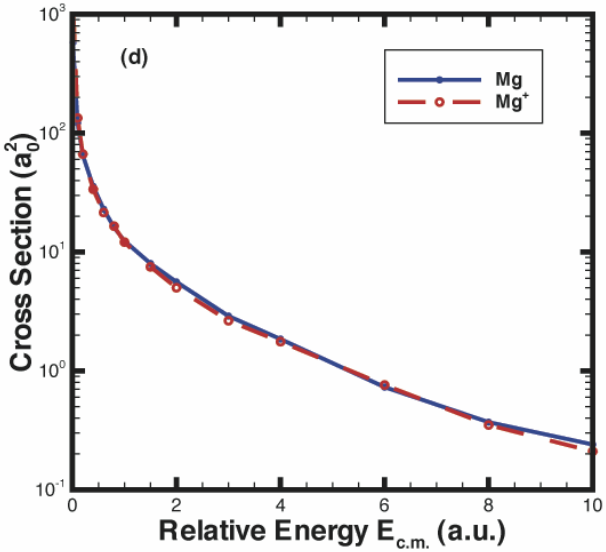

$\overline{p}$ + Ne
ionization without capture
E=2.00
E=3.00
E=4.00
E=6.00
E=10.0
E=15.0
E=25.0
Distribution
0
0.1
0.2
0.3
0.4
0.5
0
30
60
90
120
150
180
Antiproton scattering angle (deg)

Capture of antiprotons by some (radioactive) atoms and their ions



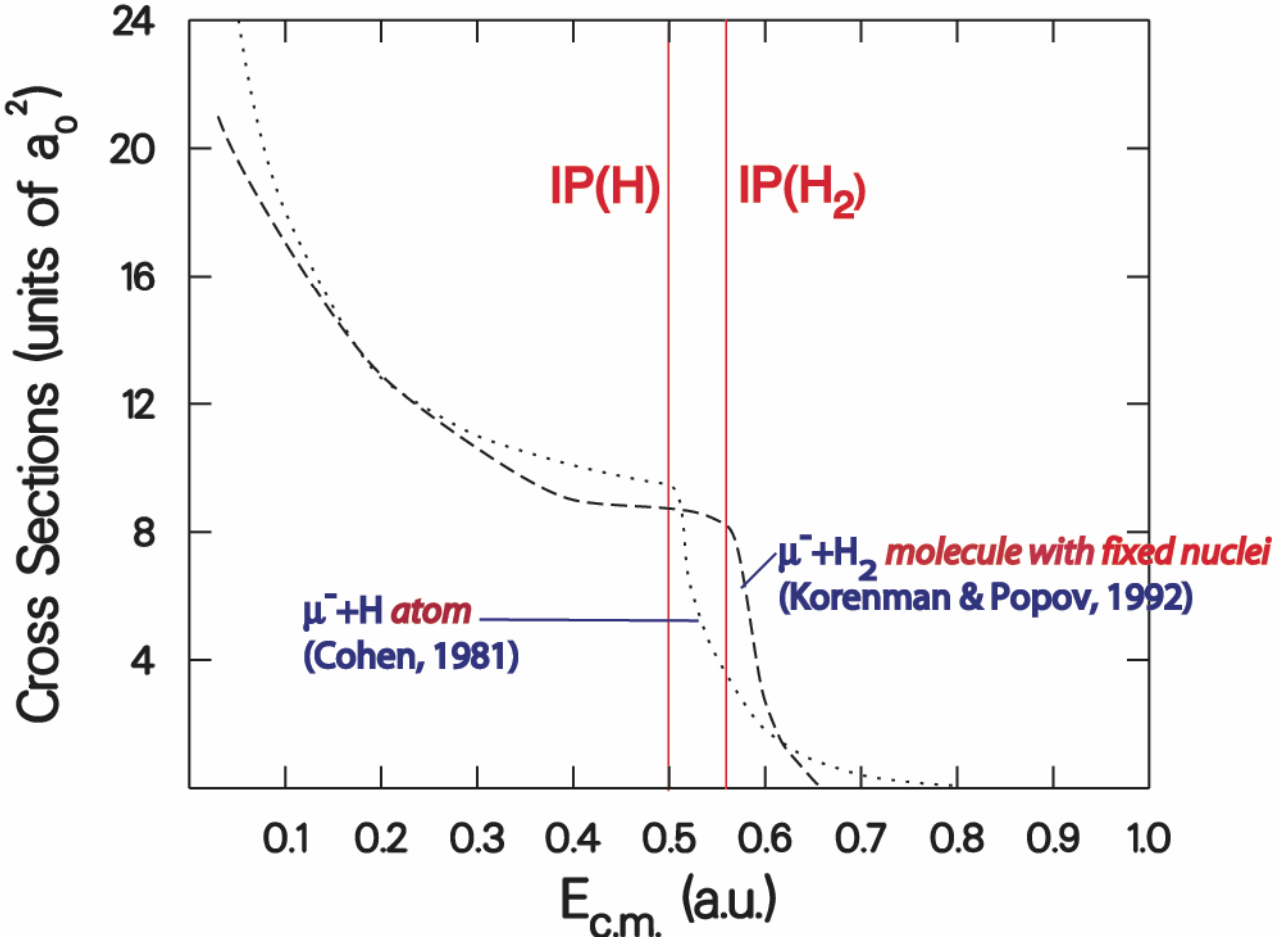


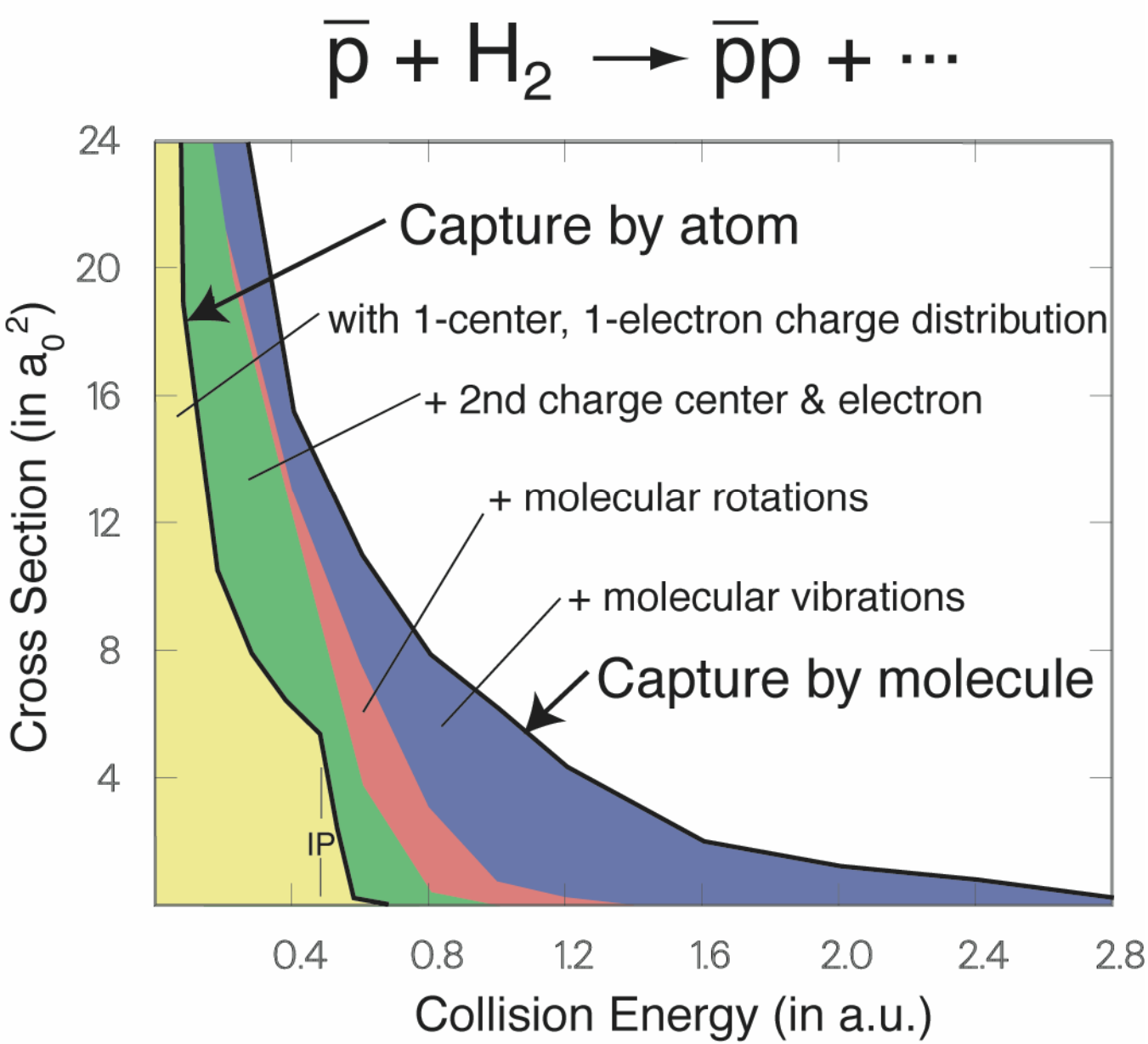


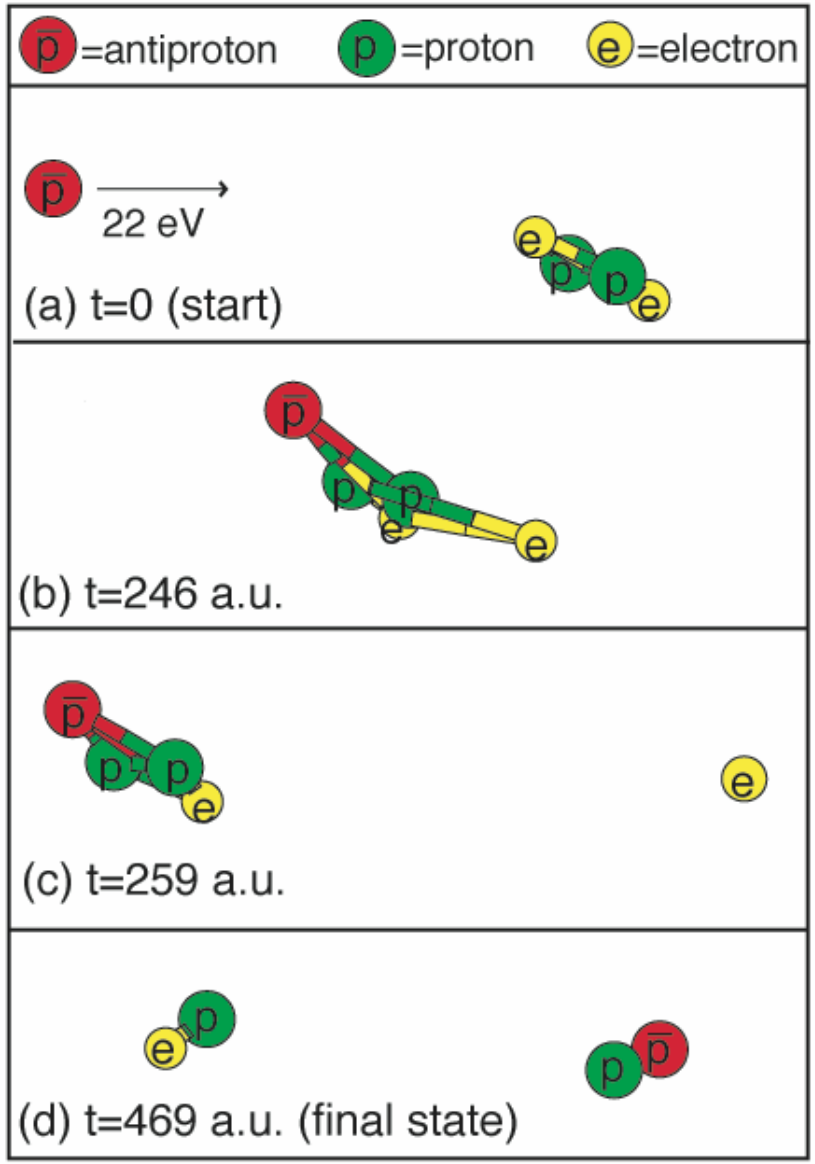


Diabatic calculations

ignoring the internal structure of the molecule



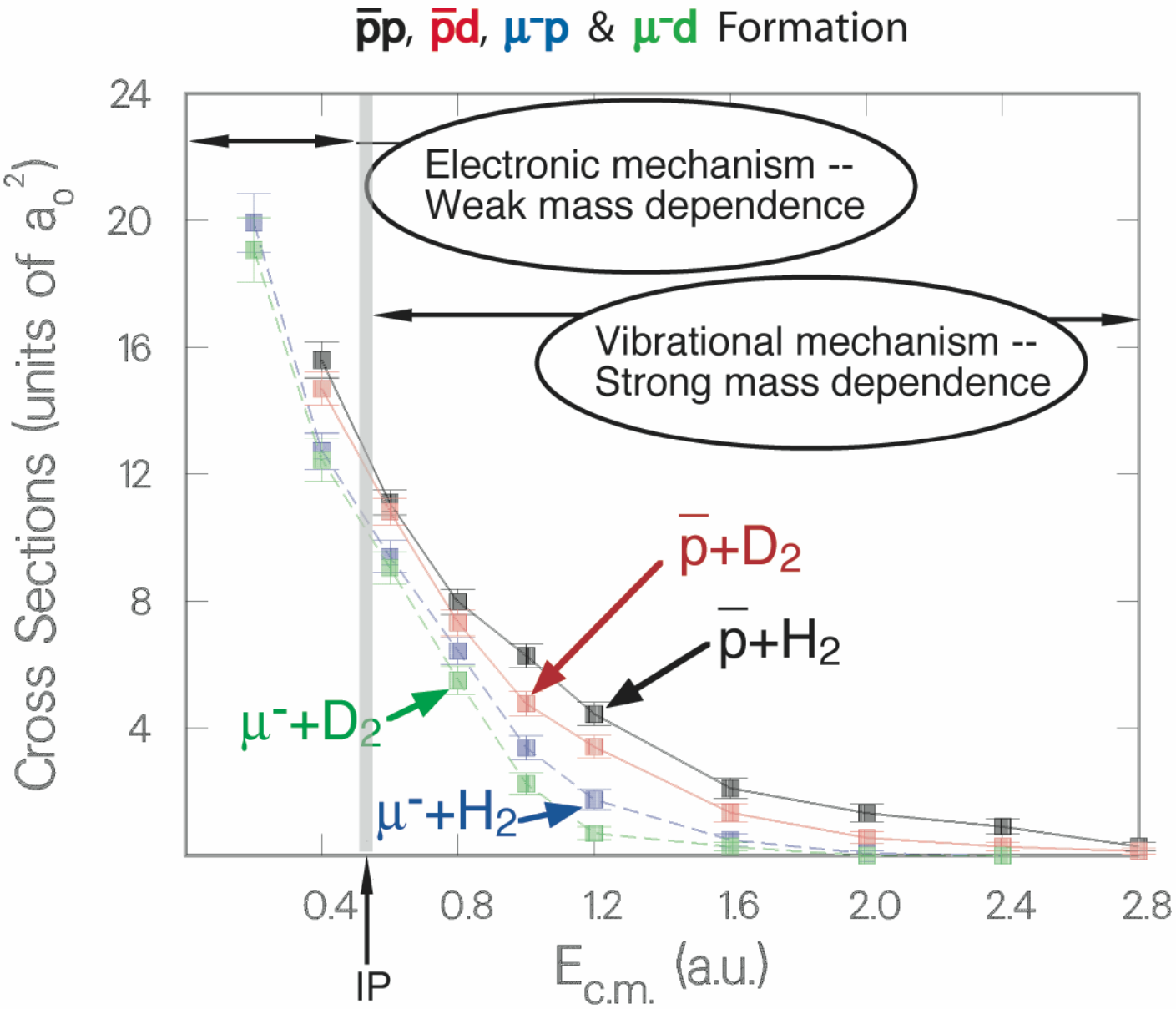

$\bar{p} + H_2 \rightarrow \bar{p}p + \cdots$
Capture by atom
with 1-center, 1-electron charge distribution
+ 2nd charge center & electron
+ molecular rotations
+ molecular vibrations
Capture by molecule
IP
Cross Section (in a_0^2)
24
20
16
12
8
4
0.4
0.8
1.2
1.6
2.0
2.4
2.8
Collision Energy (in a.u.)


p̄ =antiproton
p =proton
e =electron
p̄
22 eV
(a) t=0 (start)
e
p
p
e
p̄
p
p
e
e
(b) t=246 a.u.
p̄
p
p
e
e
(c) t=259 a.u.
e
p
e
p
p̄
(d) t=469 a.u. (final state)

Final Arrangements in $\bar{p}$+H_2 Reaction

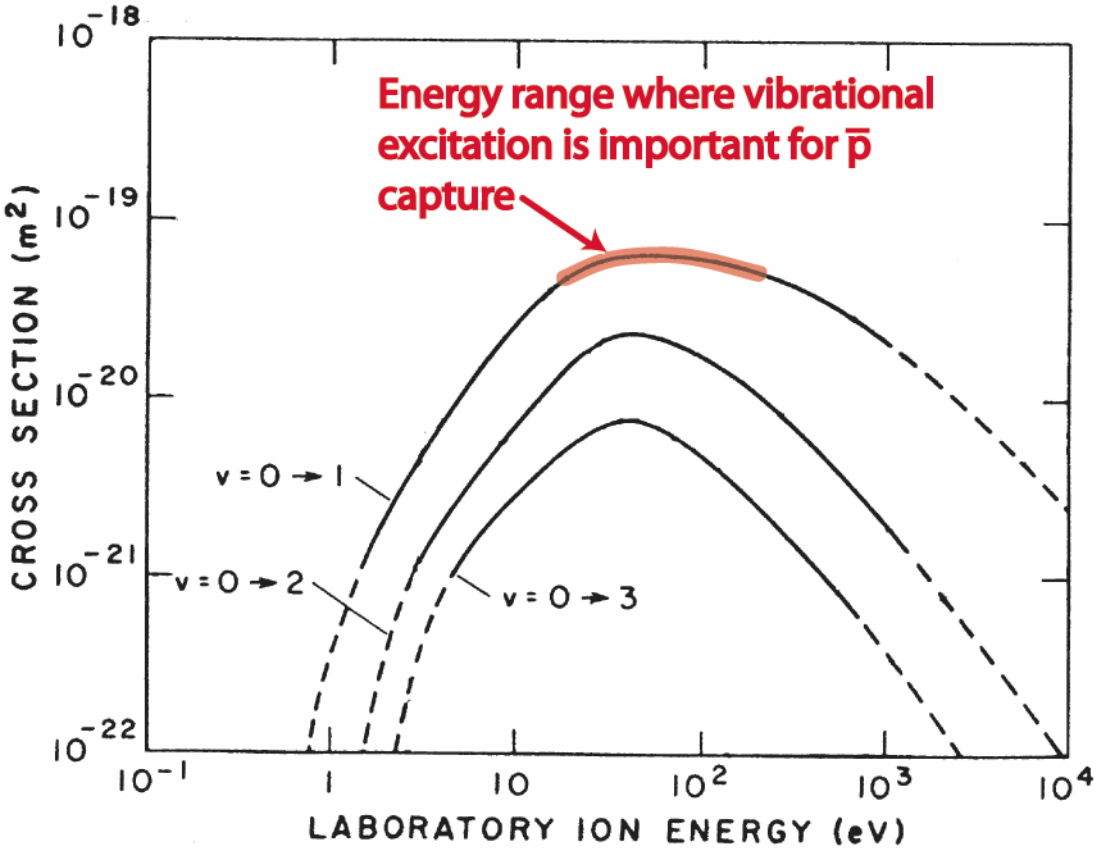
In capture of $\bar{p}$ by H_2, intermediate states such as $pp\bar{p}e^-$ or $p\bar{p}e^-$ are possible, but are predissociative and/or autoionizing. For this reason we have adopted the approach of following the trajectories long enough that the isolated $\bar{p}p$ atom can be characterized. The reactions distinguished are then

$$\bar{p} + H_2 \rightarrow \begin{cases} \bar{p}p + H + e^- & \sim 98\% & \text{(a)} \\ \bar{p}p + H^- & \lesssim 2\% \text{ (mainly at low } E) & \text{(b)} \\ \bar{p}p + p + e^- + e^- & \lesssim 1\% \text{ (mainly at high } E) & \text{(c)} \end{cases}$$


p̄p, p̄d, μ⁻p & μ⁻d Formation
Cross Sections (units of a0²)
24
20
16
12
8
4
Electronic mechanism --
Weak mass dependence
Vibrational mechanism --
Strong mass dependence
p̄+D2
p̄+H2
μ⁻+D2
μ⁻+H2
0.4
0.8
1.2
1.6
2.0
2.4
2.8
IP
Ec.m. (a.u.)

Comparison with *nonexotic* physics

$p+H_2$



$E_{lab} = 1.5\ E_{c.m.}$

Adapted from Figure 1 of A.V. Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990).

Another comparison with *nonexotic* physics

"Lambert-Salter plot"

Collisional vibrational deactivation of polyatomic molecules at 300K

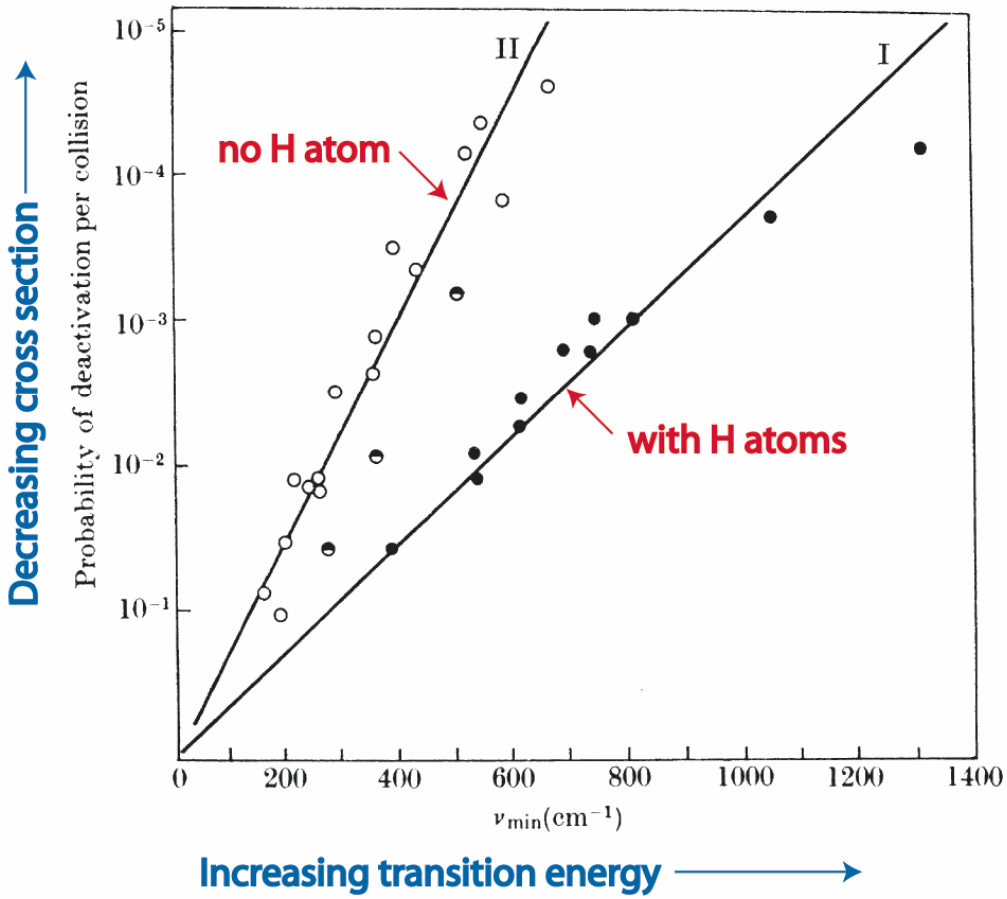


Figure 17.37 from Massey, Electronic and Ionic Impact Phenomena, vol. III

Capture of π^- in H_2+D_2 *vs* HD

P_p = Probability of initial capture by p ($P_d = 1 - P_p$)
W_p = Probability of final capture by p
$Q = (P_p - W_p)/P_p$ = Probability of transfer $\pi^- p + d \to p + \pi^- d$

Experimental: $W_p^{(H_2+D_2)} = 0.405 \pm 0.010$ ["World Fit"[a(a−d)]]
$W_p^{(HD)} = 0.338 \pm 0.008$[b]

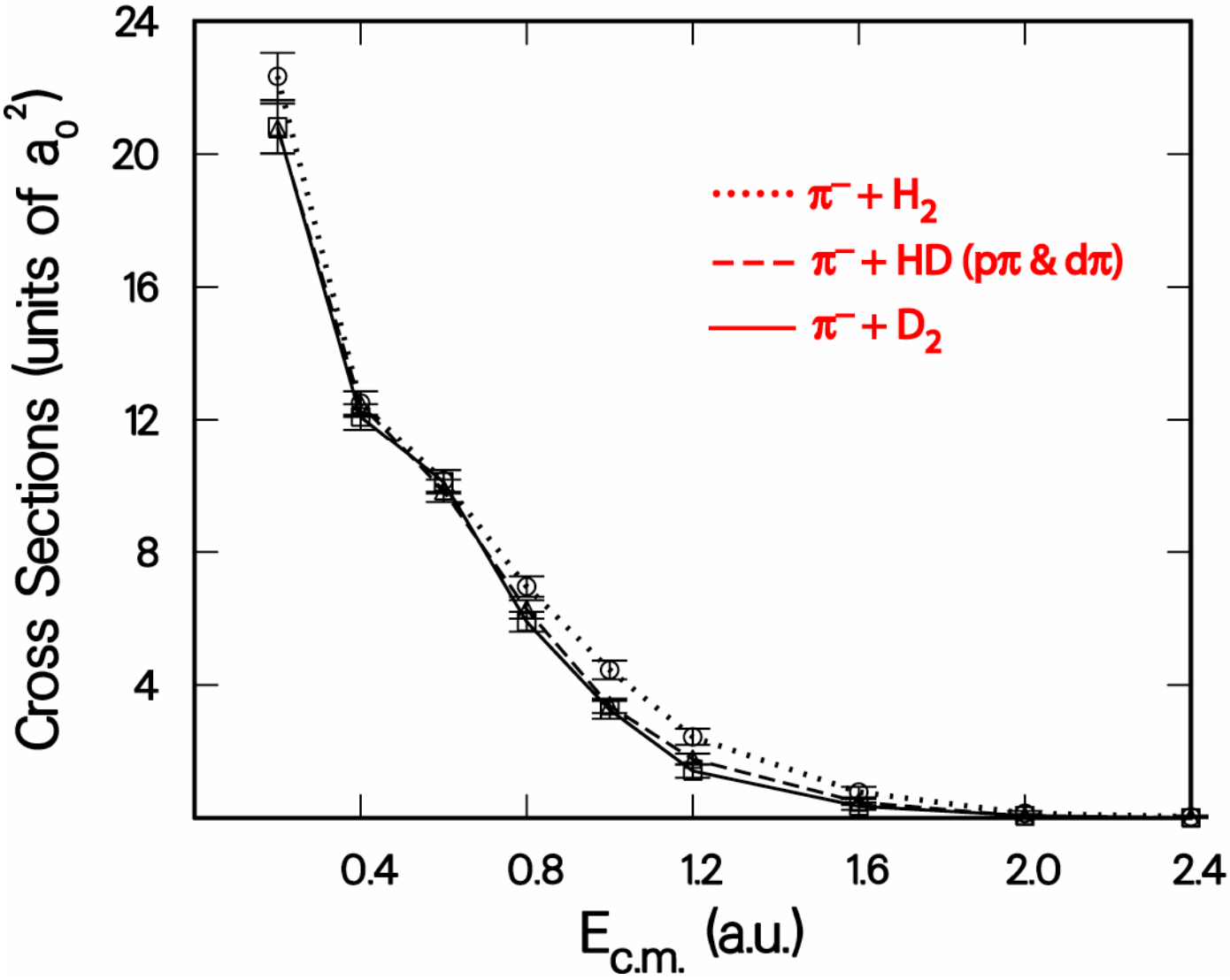
Original experimental analyses *assumed* $P_p = P_d = 0.5$ in both H_2+D_2 and HD. With this assumption:

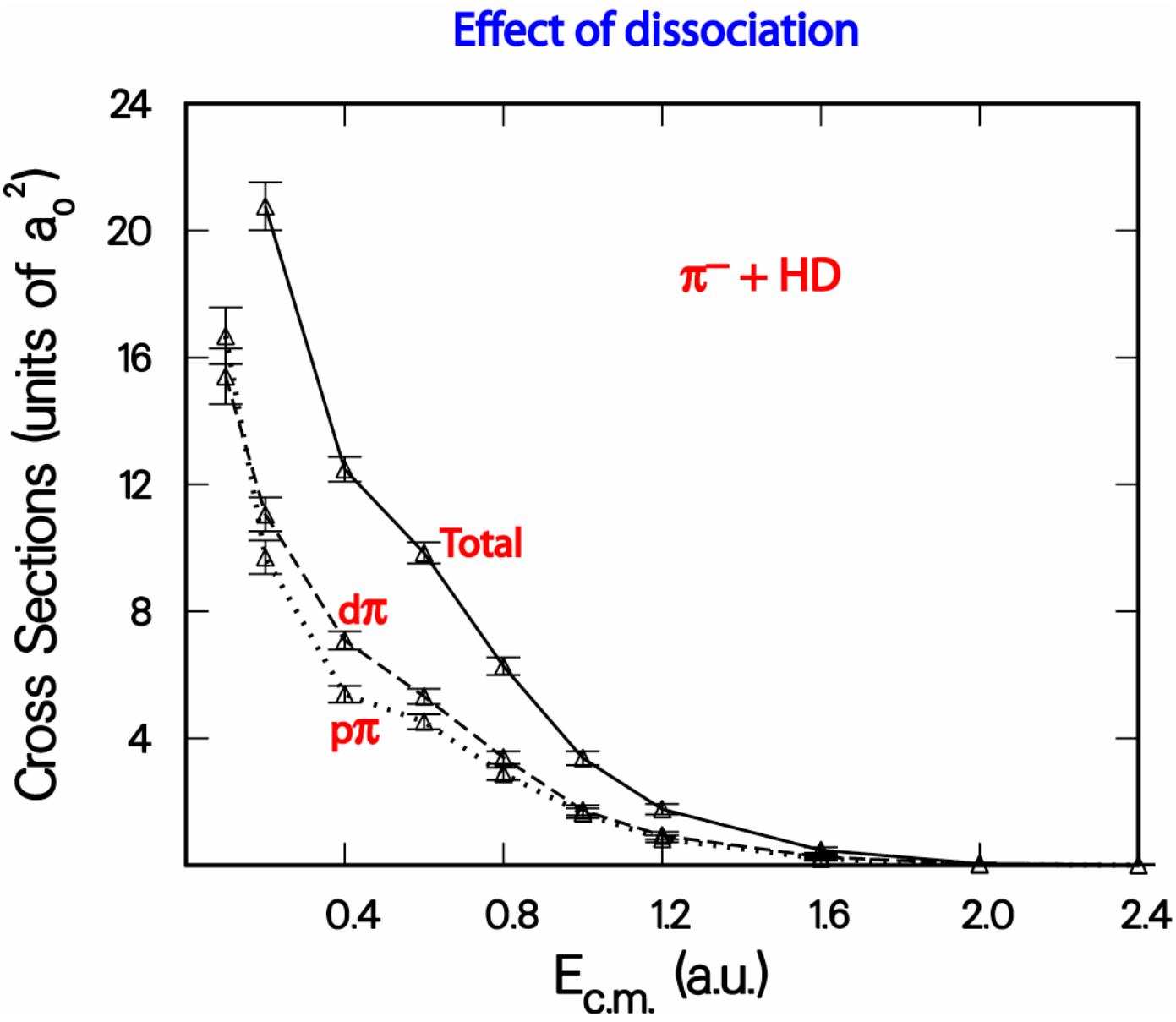
$Q = (19 \pm 2)\%$ in H_2+D_2
$Q = (32 \pm 2)\%$ in HD
} Difference was a mystery!

---

[a] Weber *et al.* (1990)
[b] Aniol *et al.* (1983)
[c] Kravtsov *et al.* (1988)
[d] Petrukhin & Prokoshkin (1969)

Negative pion capture by isotopic hydrogen molecules




Effect of dissociation
Cross Sections (units of a_0^2)
24
20
16
12
8
4
π^- + HD
Total
dπ
pπ
0.4
0.8
1.2
1.6
2.0
2.4
$E_{c.m.}$ (a.u.)

Capture of π^- in H_2+D_2 *vs* HD

P_p = Probability of initial capture by p ($P_d = 1 - P_p$)
W_p = Probability of final capture by p
$Q = (P_p - W_p)/P_p$ = Probability of transfer $\pi^- p + d \to p + \pi^- d$

Experimental: $W_p^{(H_2+D_2)} = 0.405 \pm 0.010$
$W_p^{(HD)} = 0.338 \pm 0.008$

Original experimental analyses *assumed* $P_p/P_d = 1.0$ in both H_2+D_2 and HD. With this assumption:

$Q = (19 \pm 2)\%$ in H_2+D_2
$Q = (32 \pm 2)\%$ in HD
} Difference was a mystery!

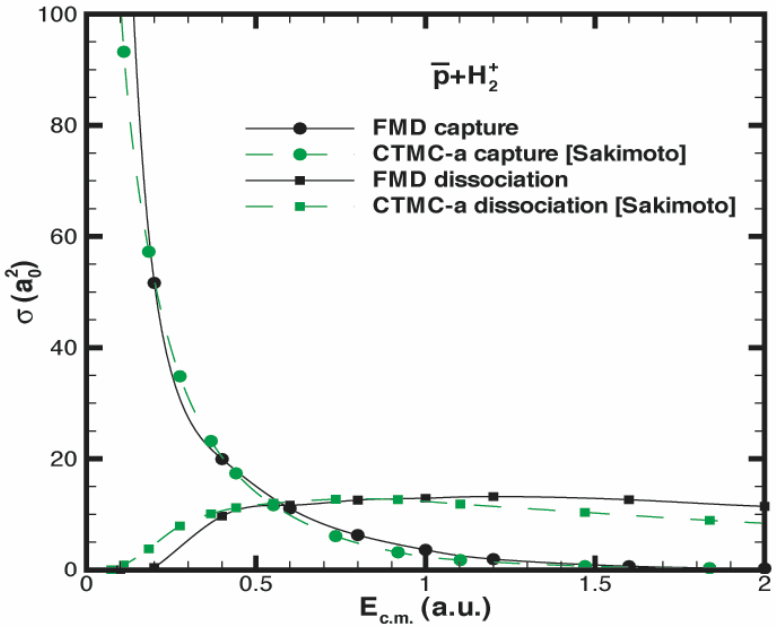
Our FMD calculations give:

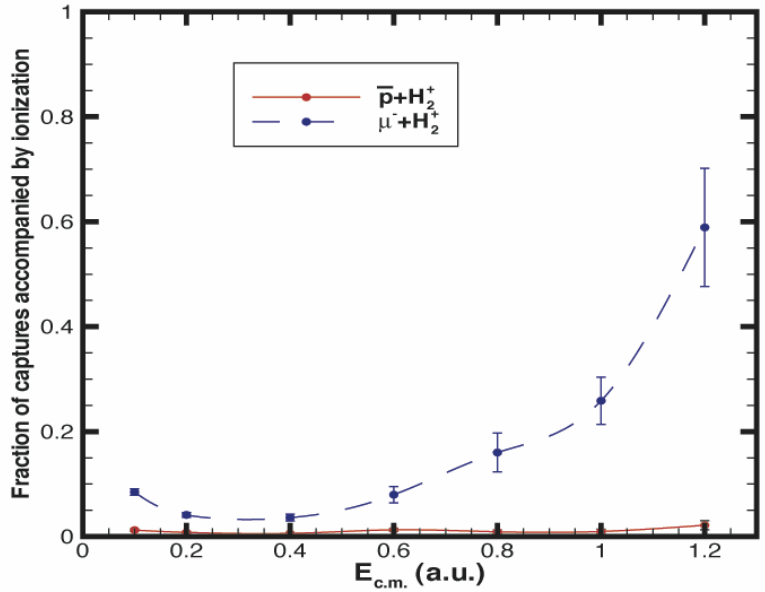
$P_p/P_d = 1.204$ in H_2+D_2
$P_p/P_d = 0.875$ in HD

With these values of P_p/P_d, the *same experimental data* implies:

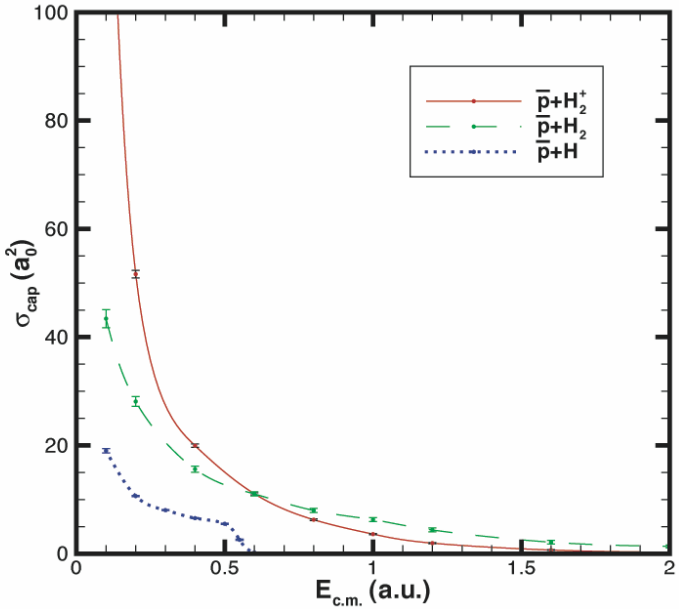
$Q = (26 \pm 2)\%$ in H_2+D_2
$Q = (28 \pm 2)\%$ in HD
} Consistency is now quite satisfactory.

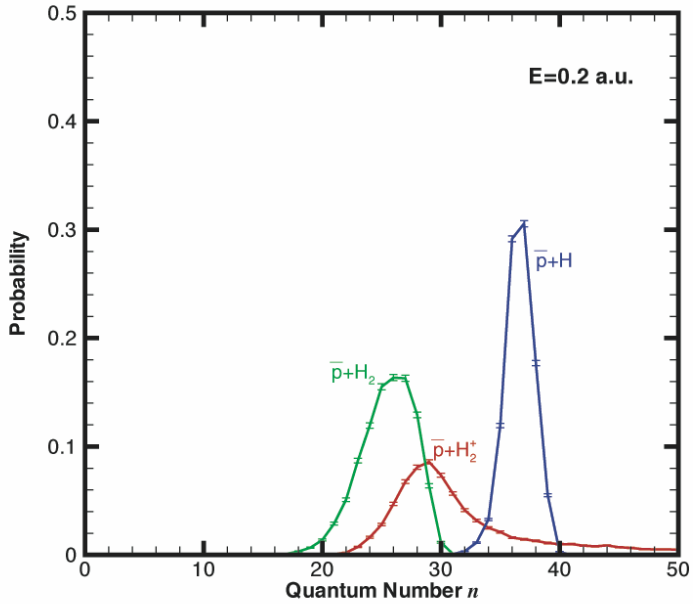
Nonadiabaticity & ionization in $\bar{p}$ capture by H_2^+





Capture of $\bar{p}$ by H, H_2 & H_2^+





Conclusions

For capture by atoms:

1. The adiabatic-ionization model is valid only for the H atom. No one-electron model can be adequate for $Z > 2$.
2. The isotope effect is quite small for atoms.
3. The initial angular momentum distribution increases more rapidly than $(2l + 1)$.

For capture by atomic ions:

1. Except for He^+, capture is similar to the parent atom.

For capture by H_2, D_2, or HD:

1. Capture cross sections are larger and extend to higher collision energies for the molecular targets than for the corresponding atomic target. This effect is greater for $\bar{p}$ than for μ^- (or π^-).
2. The isotope effect is large for H(or D)-containing molecules.
   - Initial capture favors the lighter nucleus.
   - Subsequent dissociation favors the heavier nucleus.
3. The n and l distributions are narrower and shifted to lower values relative to the distribution for the corresponding atom.

For capture by H_2^+:

1. Capture by H_2^+ is almost entirely due to target dissociation, not ionization.

Key features for verification in $\bar{p}$ capture experiments

For capture by atoms and atomic ions:

1. H and He atoms: Rather sharp cutoff at $E >$I.P.
2. Higher-Z atoms: Multiple ionization contributes to capture.
3. Atomic singly charged ions: Similar to parent atom, *except* for He.

For capture by hydrogen molecules and ions:

1. H_2 molecule: Capture at much higher energies than for H atom.
2. H_2^+ molecular ion: Capture occurs mostly without ionization.

Speculations: (based on interpretation of existing calculations)

1. Capture by molecules not containing H or D, *e.g.* O_2, may be similar to that of the constituent atoms.
2. Hydrides may be *qualitatively* like H_2. (H_2O might be interesting.)

Of great basic interest:

- Comparison of cross sections and quantum-number distributions for capture of $\bar{p}$ by H, H_2, and H_2^+.