Problems of theoretical interpretation of COLTRIMS results on ionization of helium by fast bare-ion impact

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Outline

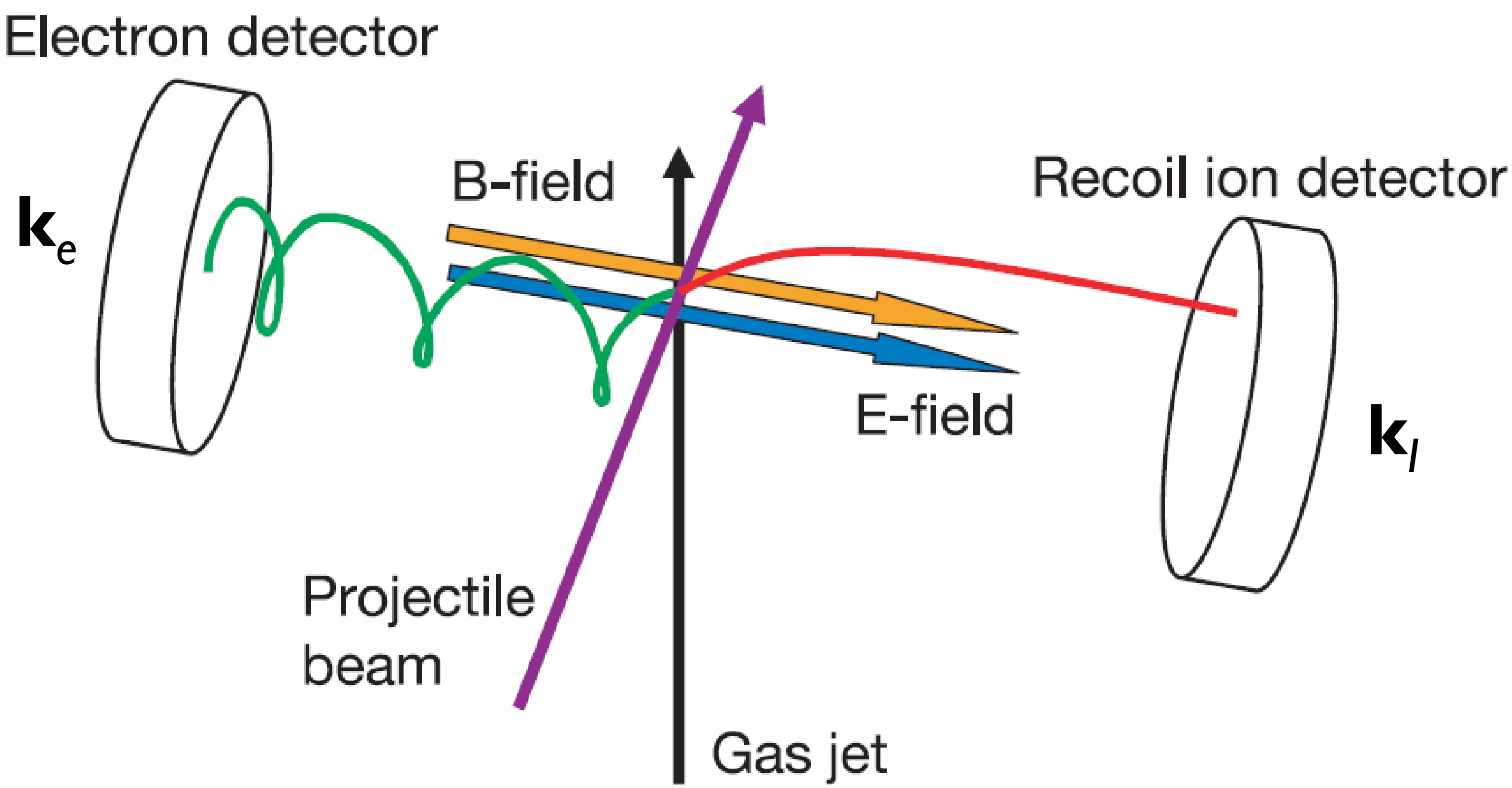
I. COLTRIMS (a reaction microscope)

II. "C^{6+} puzzle"
(100 MeV/a.m.u. $C^{6+}+He \rightarrow C^{6+}+He^{+}+e^{-}$)

III. Projectile coherence effects
(the role of the projectile's wave packet)

IV. Recent data for proton impact
(1 MeV/a.m.u. $H^{+}+He \rightarrow H^{+}+He^{+}+e^{-}$)

COLTRIMS
Cold-Target Recoil-Ion-Momentum Spectroscopy



Momentum uncertainties

- Determining energy and momentum transfers, T and $\mathbf{Q}$, using the respective conservation laws:

$$T = E_e + E_I + I - E_T \qquad (E_T, E_I << E_e, I)$$

$$\mathbf{Q} = \mathbf{k}_e + \mathbf{k}_I - \mathbf{q}_T$$

$$\Delta q_T \sim 0.15\sqrt{T_{\mathrm{He}}} \text{ a.u.}$$

(in atomic units $e=\hbar=m_e=1$ and $c=137$)

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

Three-dimensional imaging of atomic four-body processes

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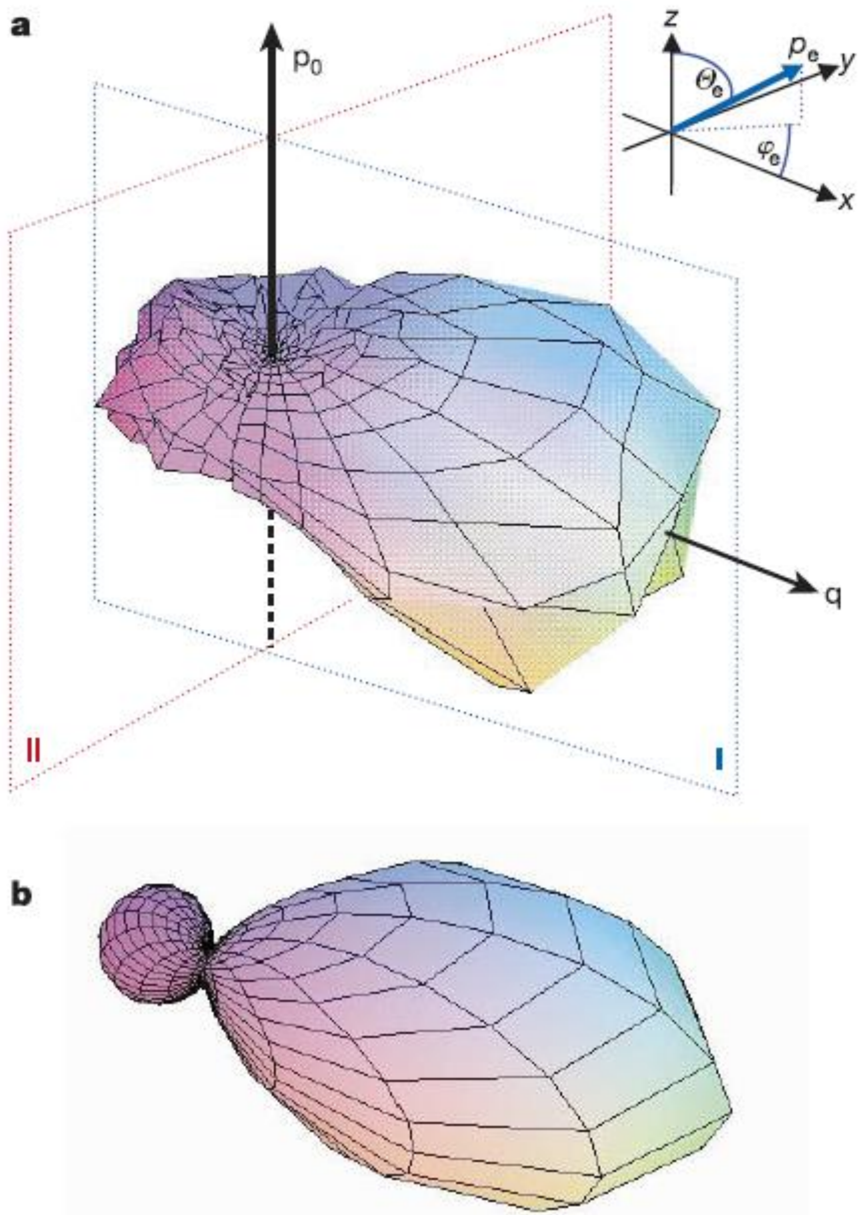
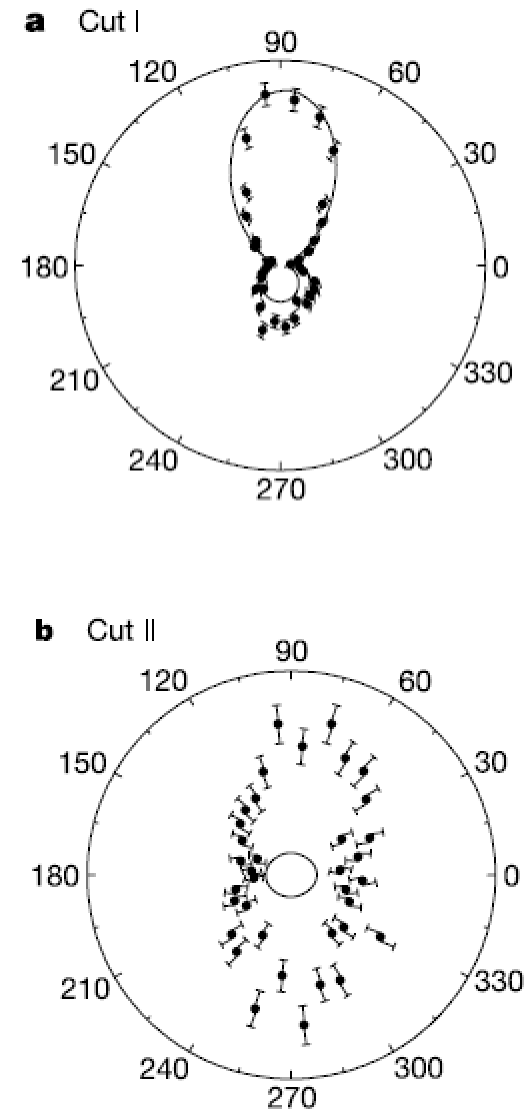
100 MeV/a.m.u. $C^{6+} + He \rightarrow C^{6+} + He^{+} + e^{-}$

at Q=0.75 a.u. and E_e=6.5 eV,

v_p = 58 a.u.

Experiment vs. Theory (CDW-HF)





Theoretical analysis of C^{6+} puzzle

- K. A. Kouzakov et al.
  "Singly ionizing 100-MeV/amu C^{6+}+He collisions with small momentum transfer"
  Phys. Rev. A **86**, 032710 (2012)
- Comment by M. Schulz et al.
  Phys. Rev. A **87**, 046701 (2013)
- Reply by K. A. Kouzakov et al.
  Phys. Rev. A **87**, 046702 (2013)

$Z_p/\upsilon_p \sim 0.1 \Rightarrow$ 1st Born approximation (FBA)

$$\mathcal{T}_{fi}^{\mathrm{FBA}} = -\frac{4\pi Z_p}{Q^2}\rho_{fi}(\mathbf{Q}) \qquad (Z_p = 6)$$

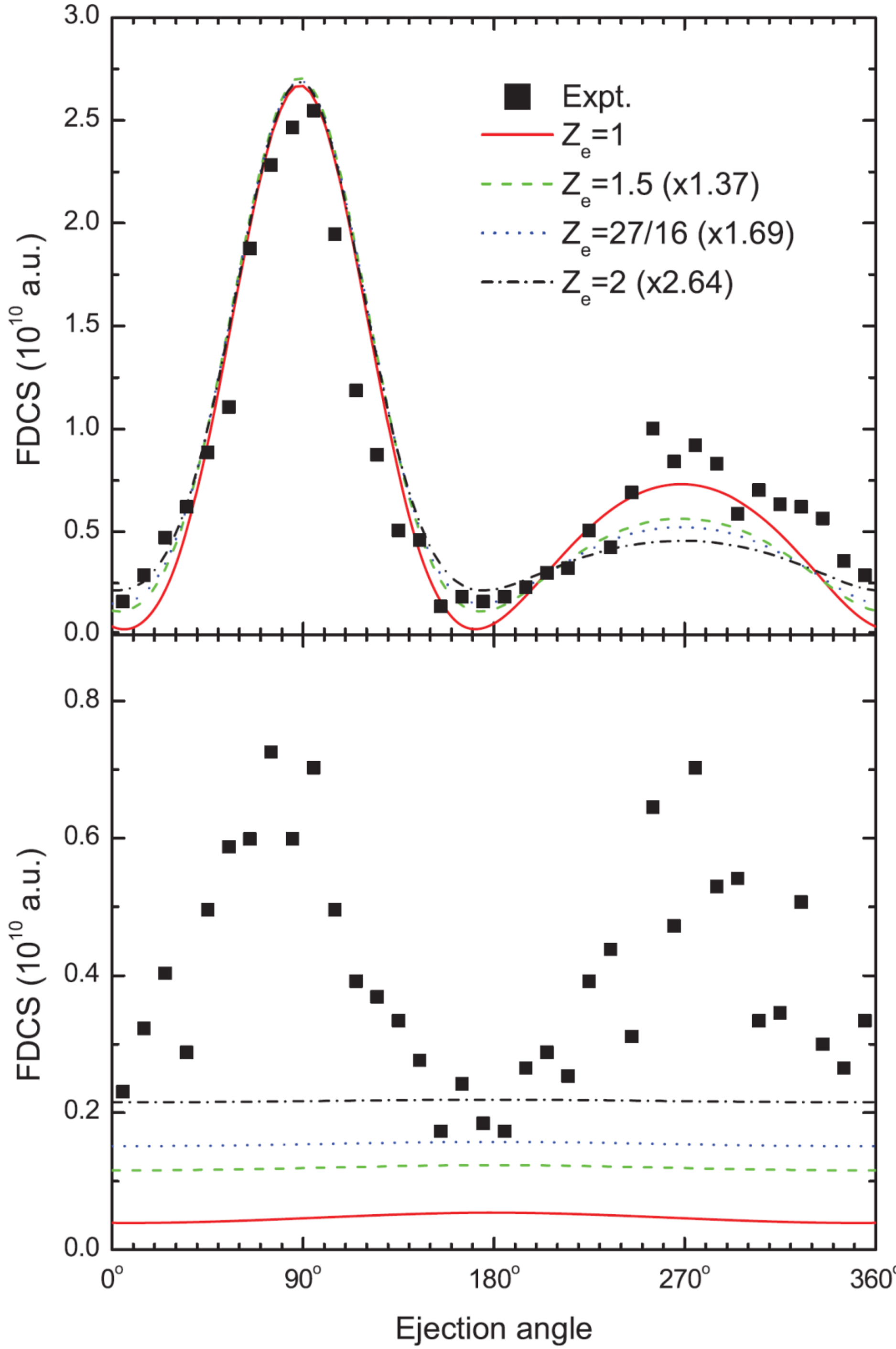
$$\rho_{fi}(\mathbf{Q}) = \langle \Psi_f | \sum_{j=1}^{2} e^{i\mathbf{Q}\cdot\mathbf{r}_j} | \Psi_i \rangle$$

$$\Psi_i(\mathbf{r}_1, \mathbf{r}_2) = \phi_{1s}(\mathbf{r}_1; Z_i)\phi_{1s}(\mathbf{r}_2; Z_i),$$

$$\Psi_f(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_{\mathbf{k}_e}^{(-)}(\mathbf{r}_1; Z_e)\phi_{1s}(\mathbf{r}_2; Z_f) + \phi_{\mathbf{k}_e}^{(-)}(\mathbf{r}_2; Z_e)\phi_{1s}(\mathbf{r}_1; Z_f)\right],$$

$$Z_i = 27/16 \text{ and } Z_f = 2,\ 1 \leqslant Z_e \leqslant 2$$

FBA vs. Experiment



Possible explanations for the failure of FBA

- Relativistic effects

(the C^{6+} velocity is almost 0.5*c*)

- Second Born effects

(FBA gives a flat angular distribution in the perpendicular plane)

- Distorted-wave effects

(due to the C^{6+}-α Coulomb interaction)

Relativistic effects

$$\mathcal{T}_{fi}^{\text{QED}} = \frac{1}{c^2} D_{\mu\nu}(q^2) J_{fi}^{\mu}(-q) J_{kk'}^{\nu}(q), \quad q = (T, \mathbf{Q})$$

$$\mathcal{T}_{fi}^{\text{QED}} = \frac{1}{1 - \frac{T^2}{Q^2 c^2}} \sqrt{\frac{E_p}{E'_p}} \left[1 - \frac{\mathbf{v}_p \cdot \mathbf{j}_{fi}(\mathbf{Q})}{c^2 \rho_{fi}(\mathbf{Q})} \right] \mathcal{T}_{fi}^{\text{FBA}},$$

$$\rho_{fi}(\mathbf{Q}) = \langle \Psi_f | \sum_{j=1}^{2} e^{i\mathbf{Q}\cdot\mathbf{r}_j} | \Psi_i \rangle,$$

$$\mathbf{j}_{fi}(\mathbf{Q}) = -\frac{i}{2} \langle \Psi_f | \sum_{j=1}^{2} (e^{i\mathbf{Q}\cdot\mathbf{r}_j} \nabla_j + \nabla_j e^{i\mathbf{Q}\cdot\mathbf{r}_j}) | \Psi_i \rangle$$

$$\mathbf{j} = (\rho\mathbf{v} + \mathbf{v}\rho)/2$$

$$\frac{\mathbf{v}_p \cdot \mathbf{j}_{fi}(\mathbf{Q})}{c^2 \rho_{fi}(\mathbf{Q})} \sim \frac{v_p v_a}{c^2}$$

$v_p/c \approx ½$ but $v_a/c << 1$.

The Lorentz factor is about $\gamma \approx 1.1$. It means scaling up of the FDCS by a factor of about 1.2.

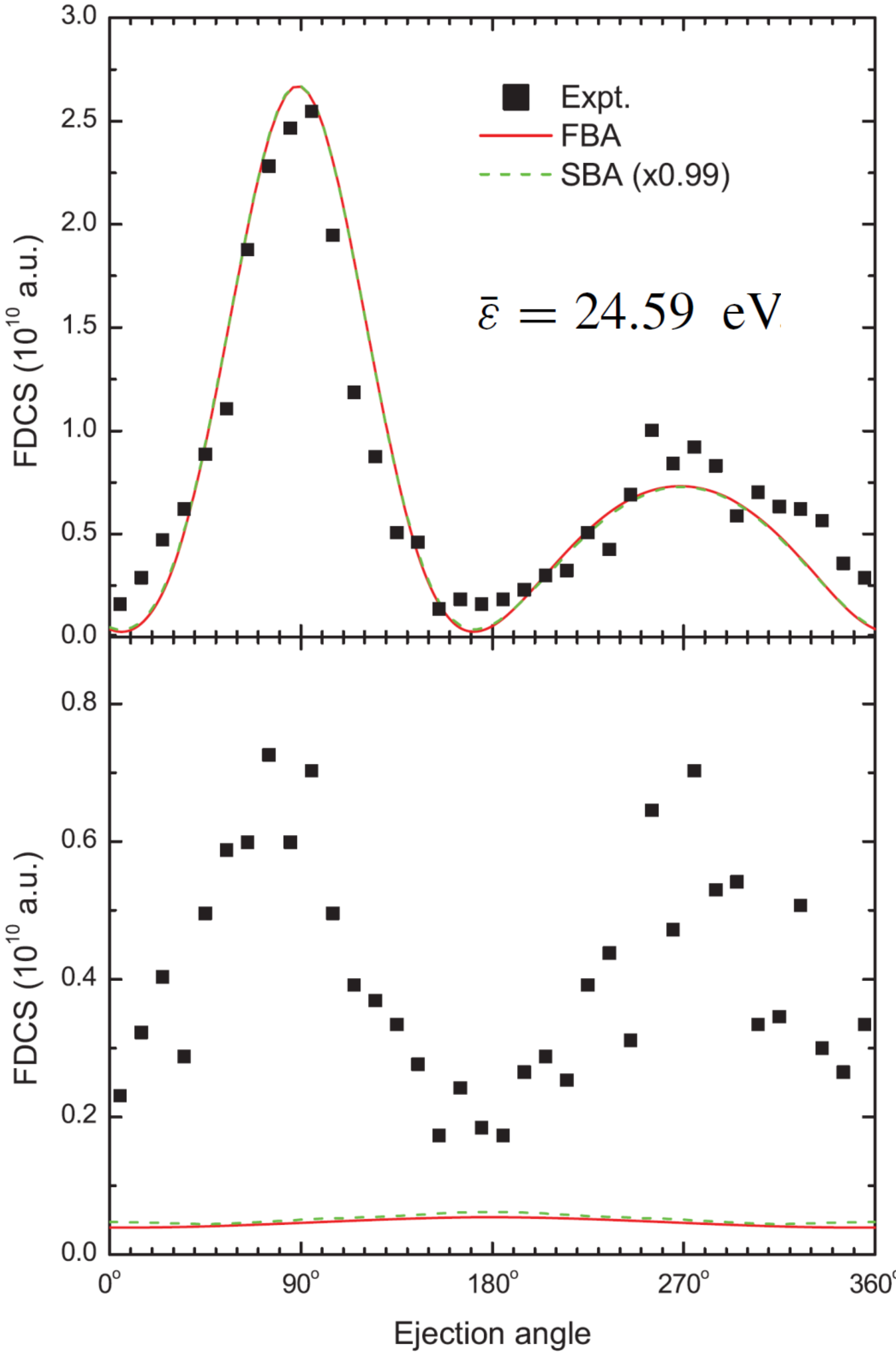
Second Born effects

$$\mathcal{T}_{fi}^{\mathrm{SBA}} = \mathcal{T}_{fi}^{\mathrm{FBA}} + \delta\mathcal{T}_{fi}^{\mathrm{SBA}},$$

$$\delta\mathcal{T}_{fi}^{\mathrm{SBA}} = \sum_n \int \frac{d^3p}{(2\pi)^3} \frac{4\pi Z_p}{(\mathbf{Q}-\mathbf{p})^2} \frac{4\pi Z_p}{p^2} \times \frac{[\rho_{fn}(\mathbf{Q}-\mathbf{p}) - 2\delta_{fn}][\rho_{ni}(\mathbf{p}) - 2\delta_{ni}]}{\mathbf{v}_p \cdot \mathbf{p} + \varepsilon_i - \varepsilon_n + i0}.$$

$$\delta\mathcal{T}_{fi}^{\mathrm{SBA}} = \int \frac{d^3p}{(2\pi)^3} \frac{4\pi Z_p}{(\mathbf{Q}-\mathbf{p})^2} \frac{4\pi Z_p}{p^2} \times \frac{\rho_{fi}(\mathbf{Q}) - 2\rho_{fi}(\mathbf{Q}-\mathbf{p}) - 2\rho_{fi}(\mathbf{p}) + g_{fi}(\mathbf{Q},\mathbf{p})}{\mathbf{v}_p \cdot \mathbf{p} - \bar{\varepsilon} + i0},$$

$$g_{fi}(\mathbf{Q},\mathbf{p}) = \langle \Psi_f | e^{i(\mathbf{Q}-\mathbf{p})\cdot\mathbf{r}_1} e^{i\mathbf{p}\mathbf{r}_2} + e^{i(\mathbf{Q}-\mathbf{p})\cdot\mathbf{r}_2} e^{i\mathbf{p}\mathbf{r}_1} + 4 | \Psi_i \rangle.$$



SBA vs. Experiment

Distorted-wave effects

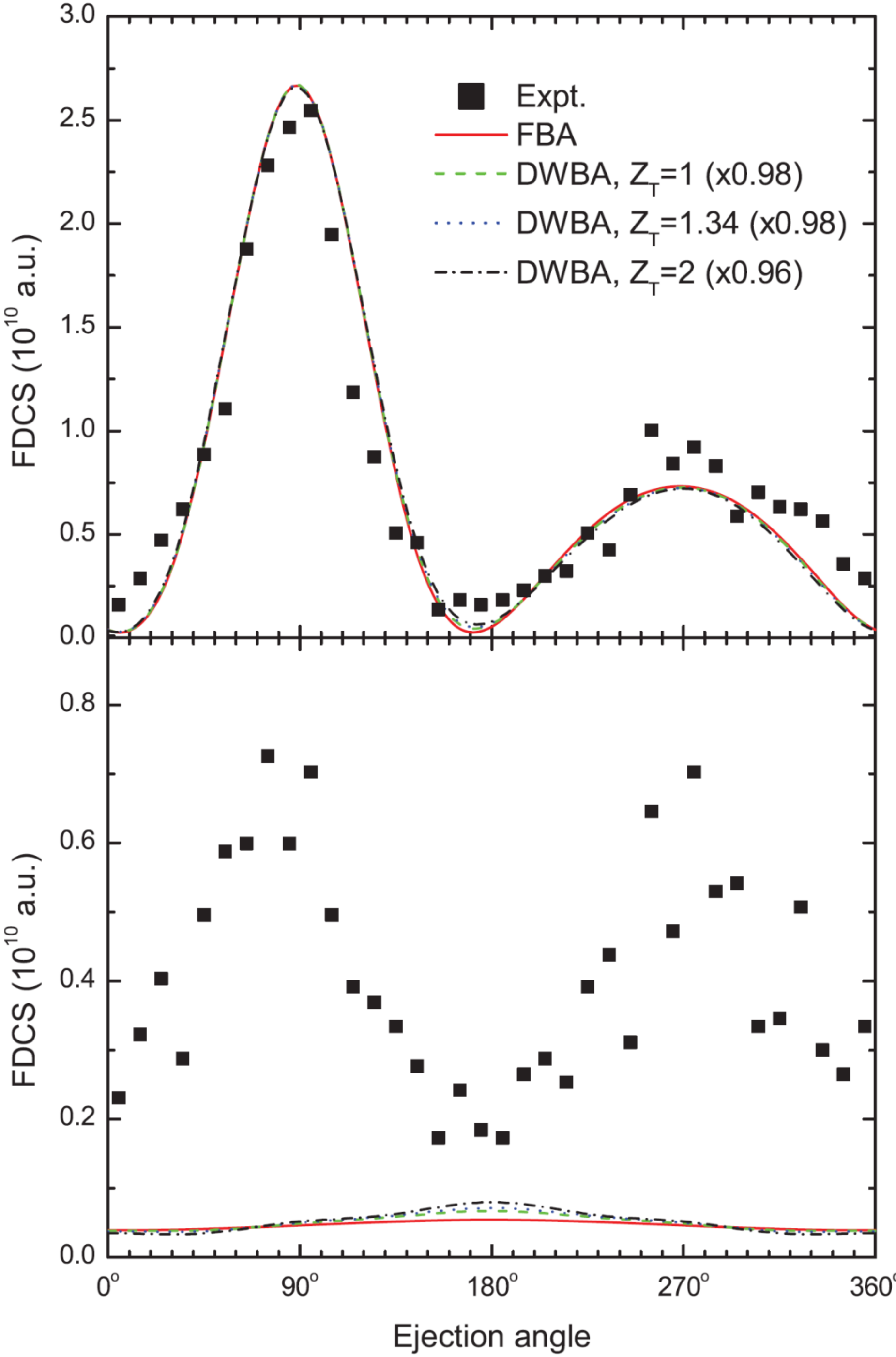
$$\mathcal{T}_{fi}^{\mathrm{DWBA}} = -\left\langle \psi_{\mathbf{k}'_p}^{(-)} \Psi_f \right| \frac{Z_p}{|\mathbf{r}_1 - \mathbf{R}|} + \frac{Z_p}{|\mathbf{r}_2 - \mathbf{R}|} \left| \psi_{\mathbf{k}_p}^{(+)} \Psi_i \right\rangle,$$

Glauber or eikonal approximation

$$\mathcal{T}_{fi}^{\mathrm{DWBA}} = \int d^2 b \, (v_p b)^{2i\eta} \int \frac{d^2 q}{(2\pi)^2} \, e^{i\mathbf{q}\cdot\mathbf{b}} \, \mathcal{T}_{fi}^{\mathrm{FBA}}(\mathbf{Q} - \mathbf{q})$$

$$\eta = \frac{Z_p Z_T}{\upsilon_p},$$

$$Z_p = 6, \qquad 1 \le Z_T \le 2.$$



DWBA vs. Experiment

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(the C^{6+} velocity is almost 0.5*c*)

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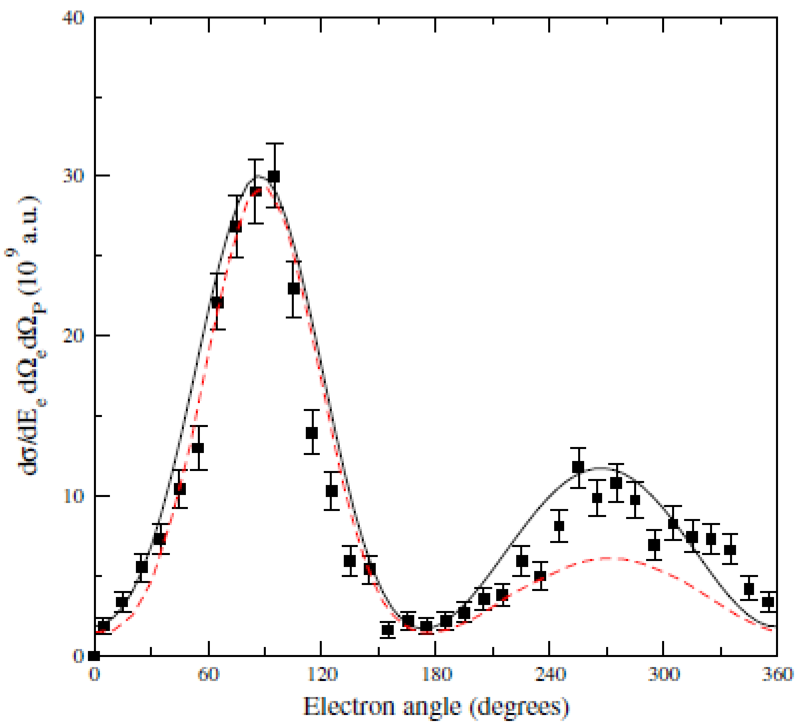
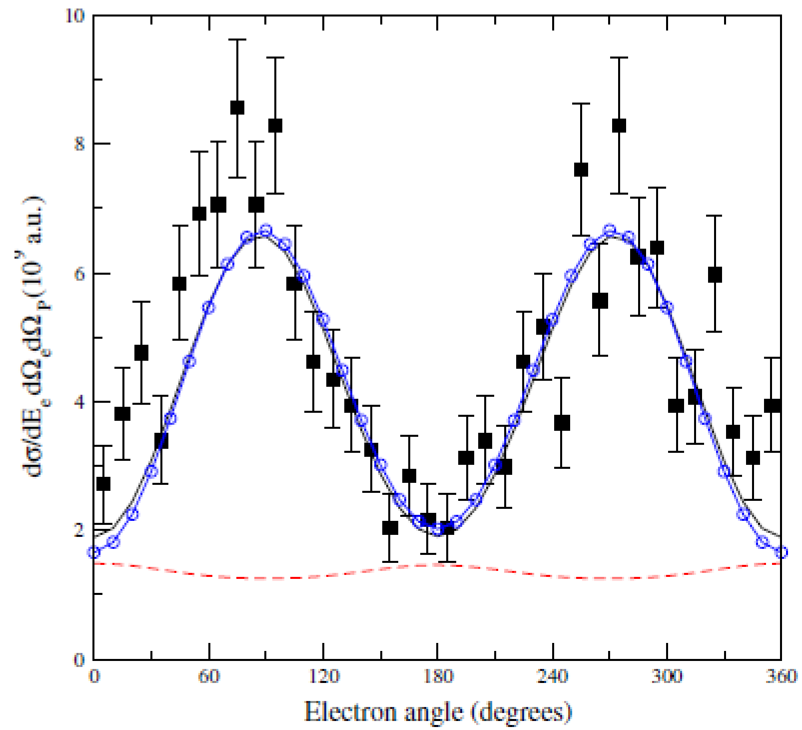
(due to the C^{6+}-α Coulomb interaction)

Finite momentum resolution

J. Fiol *et al*, J. Phys. B **39**, L285 (2006)

$\mathbf{Q} = \mathbf{k}_e + \mathbf{k}_I - \mathbf{q}_T$, $<\Delta q_T>\sim 0.15\sqrt{T_{\mathrm{He}}}$ a.u.





M. Dürr *et al* [PRA **75**, 062708 (2007)] refuted the results of J. Fiol *et al*

Comments from Michael Schulz:

- Fiol et al work with T_{He}=16 K (which would correspond to a momentum resolution of 1.3 a.u.!). But that is a ridiculous value, the real temperature in the experiment was about 1 - 2 K (ΔQ_x = 0.23 a.u., ΔQ_y=0.46 a.u.).

Comments from Masahiko Takahashi:

- I have tried to contact a Japanese researcher who has measured velocity spreads and mean velocities of neutral atomic beams, such as He, Ne, Kr, and Ar… the observed lowest temperature, among his data, relating to velocity spread is 17 K.

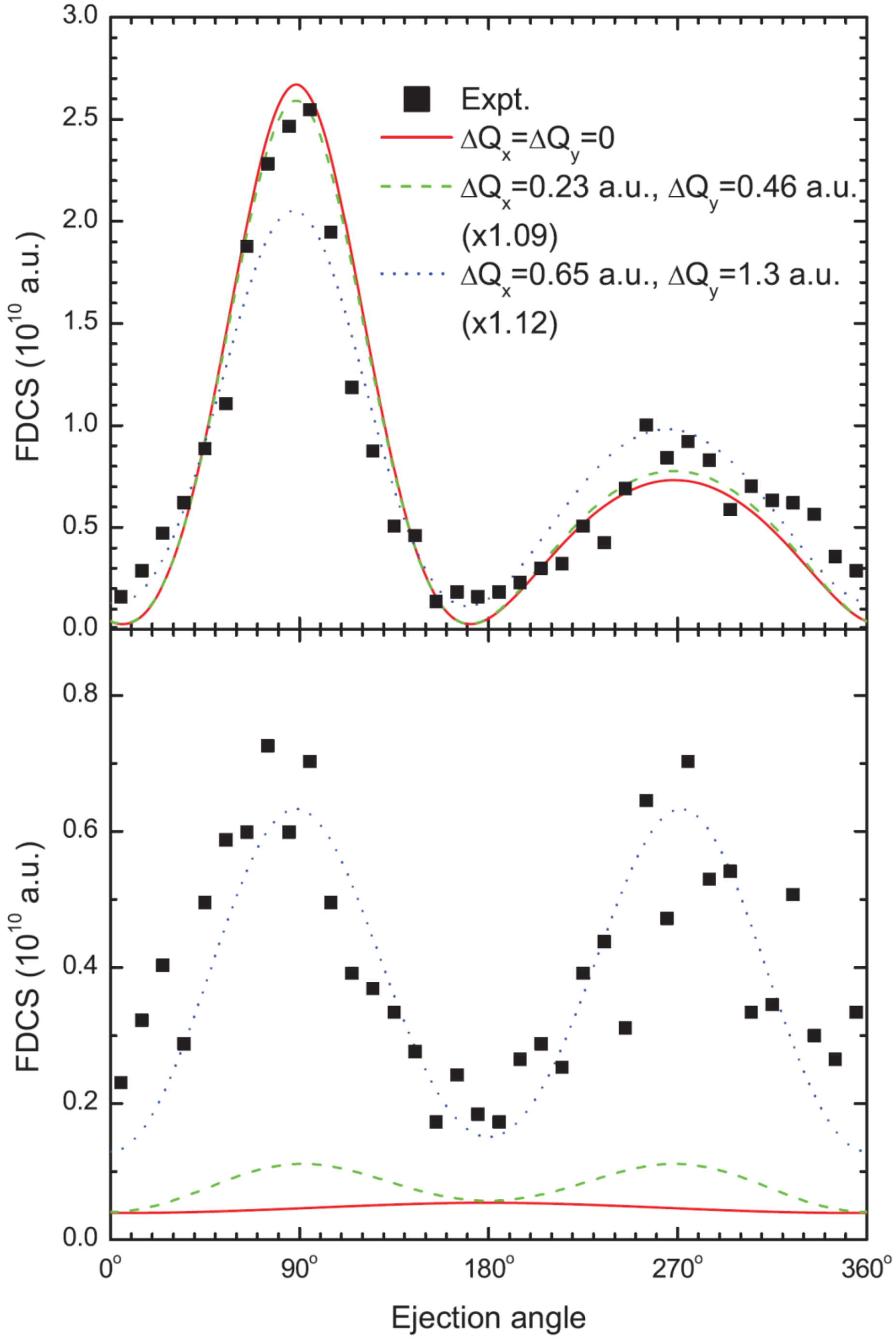
Convolution with experimental uncertainties

$$\frac{d^3\sigma}{dE_e d\Omega_e d\Omega_p} = \int_{-\infty}^{\infty} dQ'_x \int_{-\infty}^{\infty} dQ'_y \, P(Q'_x, Q'_y) \times \frac{k_e E'^2_p}{(2\pi)^5 c^4} \frac{k'_p}{k_p} \left| \mathcal{T}_{fi}^{\mathrm{FBA}} \right|^2,$$

$$\mathbf{k}'_p = \mathbf{k}_p - \mathbf{Q}', \ \ E'_p = c^2\sqrt{k'^2_p + M_p^2 c^2}$$

$$P(Q'_x, Q'_y) = \frac{1}{2\pi\sigma_x\sigma_y} \exp\left[-\frac{(Q'_x - Q_x)^2}{2\sigma_x^2} - \frac{(Q'_y - Q_y)^2}{2\sigma_y^2} \right]$$

$$\sigma_{x(y)} = \frac{\Delta Q_{x(y)}}{2\sqrt{2\ln 2}}$$



Convoluted FBA vs. Experiment

Conclusions of our analysis

- No well-established theory explains the "C^{6+} puzzle"
- There are indications that the "C^{6+} puzzle" can be due to momentum spread of the He atoms
- New, independent measurements are needed

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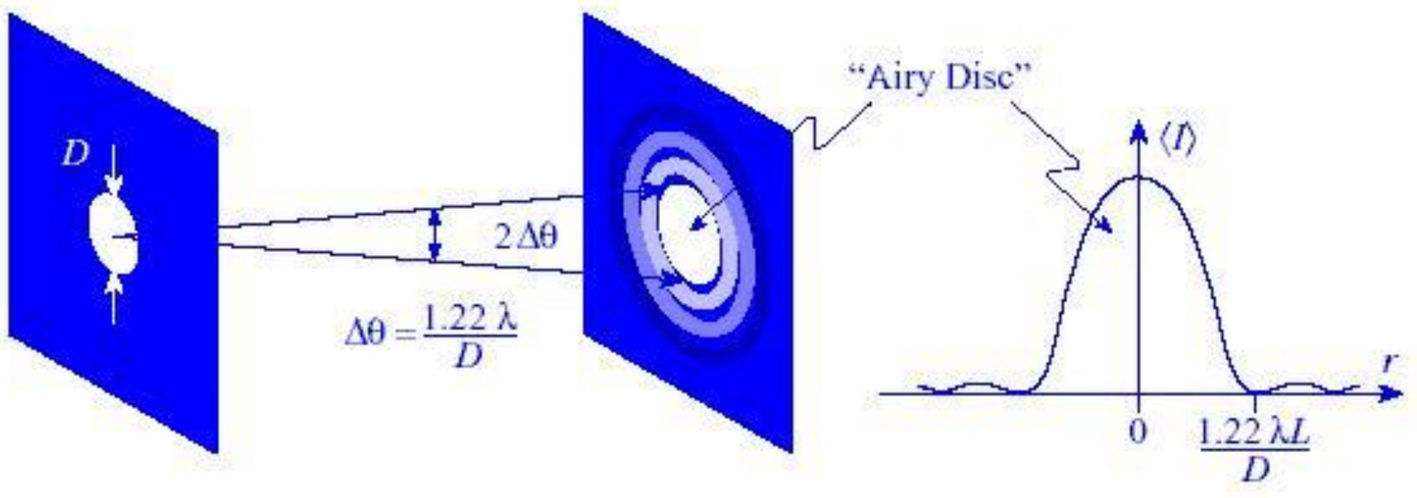
Comment on our analysis by M. Schulz *et al*, Phys. Rev. A **87**, 046701 (2013)

i. The experimental resolution is responsible only for part of the discrepancies between theory and experiment.

ii. The remaining part can be explained by the finite ***projectile coherence length***

$$\Delta r \sim 10^{-3} \text{ a.u.}$$

Diffraction of projectile beam



$$\Delta r \approx 10^{-3}\,\text{a.u.}$$

This value is by orders of magnitude smaller than the atomic size!

Time-dependent scattering theory

$$d\sigma = \frac{d\mathbf{k}_e}{(2\pi)^3}\frac{d\mathbf{k}_I}{(2\pi)^3}\int\frac{d\mathbf{q}_p}{(2\pi)^3}\int\frac{d\mathbf{q}_T}{(2\pi)^3}\frac{2\pi}{v_z(\mathbf{q}_p)}\delta(E_e + I_1 - \mathbf{v}(\mathbf{q}_p)\cdot\mathbf{Q}(\mathbf{q}_T))|\mathcal{T}_{fi}|^2|\Phi_p(\mathbf{q}_p)|^2|\Phi_T(\mathbf{q}_T)|^2,$$

$$\mathbf{Q}(\mathbf{q}_T) = \mathbf{k}_e + \mathbf{k}_I - \mathbf{q}_T$$

$$\mathbf{v}(\mathbf{q}_p) = c\mathbf{q}_p/\sqrt{q_p^2 + M_p^2c^2}$$

$$\int \frac{d\mathbf{q}_p}{(2\pi)^3}\mathbf{q}_p|\Phi_p(\mathbf{q}_p)|^2 = \mathbf{k}_p$$

Projectile wave packet

$$\Phi_p(\mathbf{q}_p) = \int d\mathbf{r}\, e^{-i\mathbf{q}_p\cdot\mathbf{r}_p}\Psi_p(\mathbf{r}_p, t = 0)$$

The width in momentum space is huge:

$$\Delta p \sim 1/\Delta r \approx 10^3\,\text{a.u.}$$

But in velocity space it is small:

$$\Delta v \simeq c\Delta p/\sqrt{k_p^2 + M_p^2 c^2} \sim 0.04\,\text{a.u.}$$

$$d\sigma = \frac{d\mathbf{k}_e}{(2\pi)^3}\frac{d\mathbf{k}_I}{(2\pi)^3}\int\frac{d\mathbf{q}_p}{(2\pi)^3}\int\frac{d\mathbf{q}_T}{(2\pi)^3}\frac{2\pi}{v_z(\mathbf{q}_p)}\delta(E_e + I_1 - \mathbf{v}(\mathbf{q}_p)\cdot\mathbf{Q}(\mathbf{q}_T))|\mathcal{T}_{fi}|^2|\Phi_p(\mathbf{q}_p)|^2|\Phi_T(\mathbf{q}_T)|^2,$$

$$\mathbf{Q}(\mathbf{q}_T) = \mathbf{k}_e + \mathbf{k}_I - \mathbf{q}_T$$

$$\mathbf{v}(\mathbf{q}_p) = c\mathbf{q}_p/\sqrt{q_p^2 + M_p^2c^2}$$

$$\mathcal{T}_{fi} = \mathcal{T}_{fi}^{\mathrm{FBA}}(\mathbf{Q}(\mathbf{q}_T))$$

$$\mathcal{T}_{fi} = \mathcal{T}_{fi}^{\mathrm{SBA/DWBA}}(\mathbf{Q}(\mathbf{q}_T), \mathbf{v}(\mathbf{q}_p))$$

$\mathbf{v}(\mathbf{q}_p) = \mathbf{v}_p$ and $v_z(\mathbf{q}_p) = v_p$

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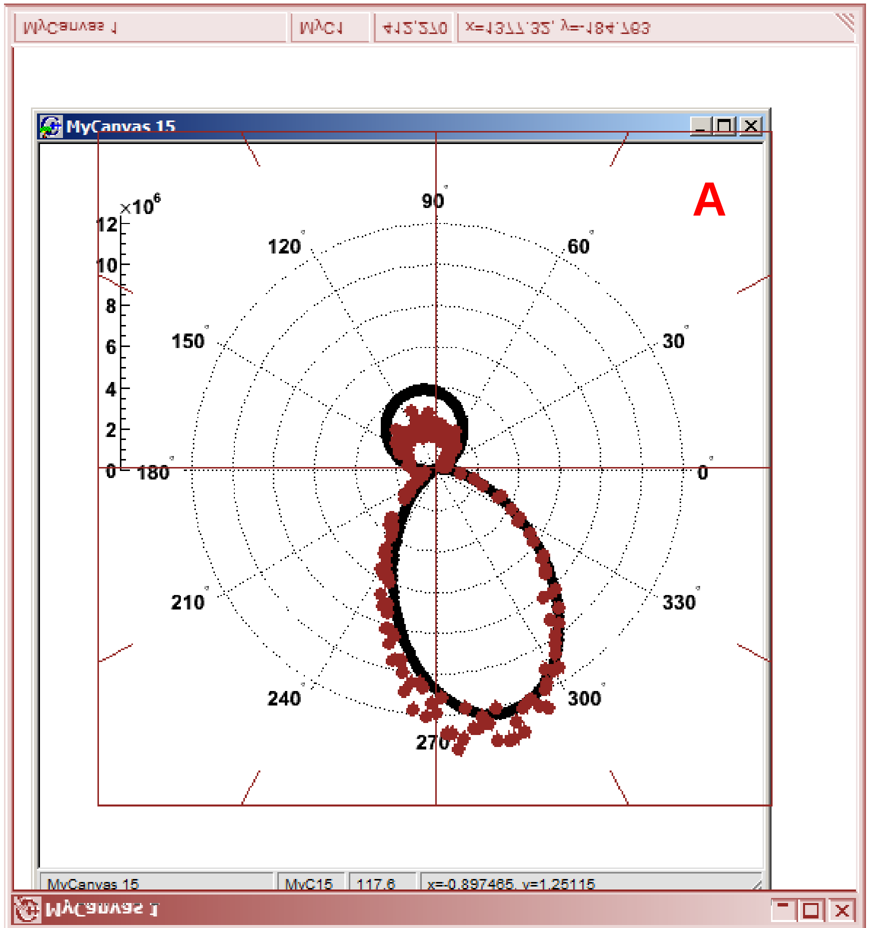
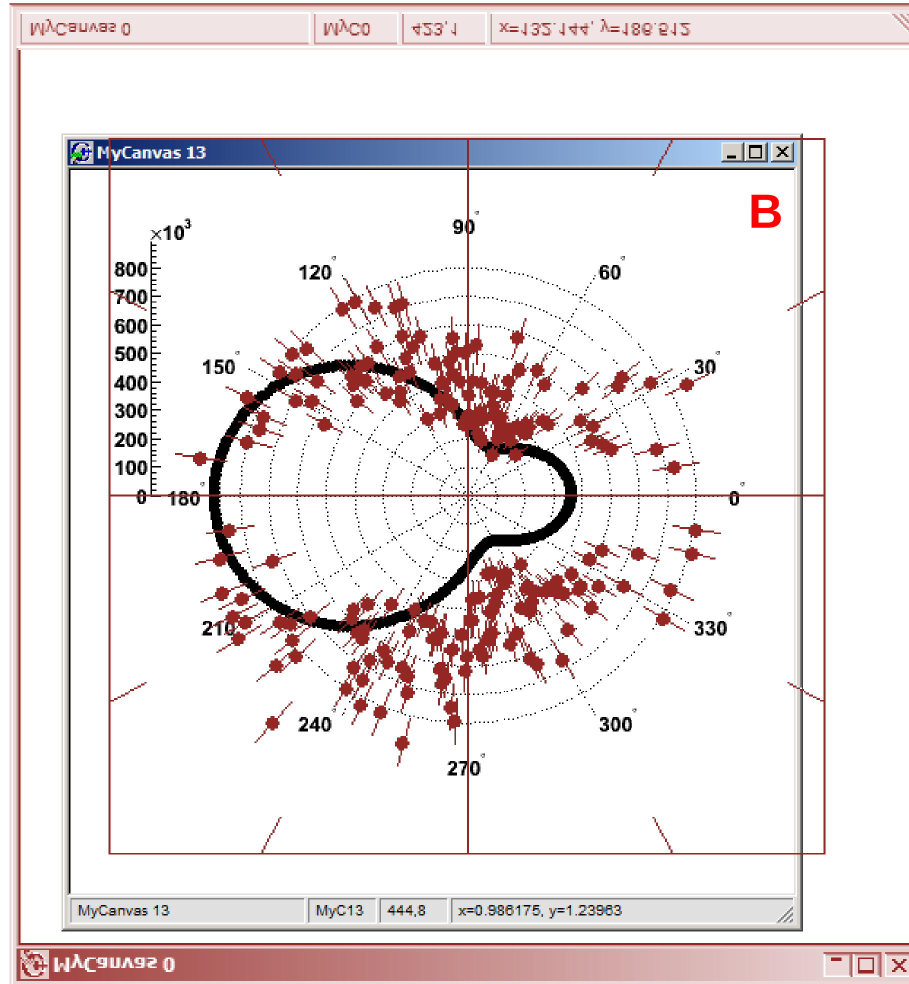
Experiment by M. S. Schöffler *et al.* (unpublished)

1 MeV/a.m.u. H^{+}+ He $\rightarrow$ H^{+}+ He^{+}+ e^{-}
at Q=0.75 a.u. and E_e=6.5 eV
(the same as in the C^{6+} case)

$v_p \approx 6$ a.u. $\Rightarrow$ $Z_p/v_p \sim 0.15$

FBA (black)
Experiment (red)
normalized to max.





THANK YOU FOR YOUR ATTENTION!